FINAL REPORT

CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM CONTRACT NO. F49620-95-C-0026

PERIOD OF PERFORMANCE: 3/1/99 - 2/29/00

Prepared For:

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH CHEMISTRY AND LIFE SCIENCES DIRECTORATE

Dr. Genevieve Haddad, Program Manager

Presented By:

UES, Inc. 4401 Dayton-Xenia Road Dayton, OH 45432-1894

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D. Conthe and Commence	falia comerce HES Inc.	stouided research evalu	ustions services for the
During the performance of	of this contract UES, Inc. p	Office of Scientific R	esearch in the areas of
Chemistry and Life Sciences Directorate, Air Force Office of Scientific Research in the areas of Polymer Chemistry, Surface Science, Theoretical Chemistry, Molecular Dynamics, Chronobiology and			
Polymer Chemistry, Surface Science, Theoretical Chemistry, Wolfectual Dynamics, Chemistry, Surface Science, Theoretical Chemistry, Wolfectual Dynamics, Chemistry, Surface Science, Theoretical Chemistry, Wolfectual Dynamics, Chemistry,			
Neural Adaptation, Perception and Cognition, Sensory Systems and Toxic Biological Interactions. Evaluations were secured for 506 AFOSR Grant Proposals. UES provided administrative tasks for			
following meeting functions: Twenty-one program reviews - 1 in the area of Chronobiology and			
Neural Adaptation; 9 in the area of Surface Science; 5 in the areas of Molecular Dynamics and			
Theoretical Chemistry; 3 in area of Polymer Chemistry; 3 in the area of Toxic Biological Interactions.			
Twelve workshops were held; 3 in the area of Chronobiology and Neural Adaptation; 3 in the area of			
Polymer Chemistry. Thirteen panel meetings were held; 8 in Molecular Dynamics and Theoretical			
Chemistry; 4 in Polymer	Chemistry and 1 in the are	ea of Chronobiology a	nd Neural Adaptation.
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INTRODUCTION

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology, Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The fourth option year effort included: 68 Proposals that were reviewed; 5 Program/Contractor Reviews; 3 Workshops and 1 Scientific Panel Meeting.

A. Evaluations of Individual Research Proposals

UES sent out 67 proposals to 206 evaluators during the performance period of 1 March 1999 through 29 February 2000.

UES has been providing to the Directorate of Chemistry and Life Sciences a Summary of Proposals under Review (SPUR) report electronically on a biweekly basis. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the AFOSR Program Managers to have a current listing of all proposal activity.

B. Contractor/Program Reviews

1. The first contractors review entitled **High Energy Density Matter (HEDM)** was held 8 June through 10 June 1999 at the Holiday Inn Cocoa Beach, Cocoa Beach, FL. The main purpose of this program is to research and develop advanced propellants containing increased energy densities to produce greater specific impulse, which will enable significantly increased payloads for rockets and missiles. With these advanced propellants, future space-bound payloads could be potentially four times greater than those of current systems for the same overall size and weight. UES provided on-site support, abstract booklets and made all arrangements for the meeting. There were 70 in attendance of which 28 were speakers. The proceedings from this contractors review were compiled and published and distributed by UES.

Dr. Michael R. Berman, Program Manger

B. <u>Contractor/Program Reviews</u> – continued

2. The first program review entitled **Tribology Program Review** was held on 14-18 June 1999 at Cheeca Lodge, Islamorada, FL. This was a joint meeting with AFOSR, the Office of Naval Research (ONR) and the National Science Foundation (NSF). The tribochemistry program is designed to provide the Air Force with improved novel lubricants, lubrication systems, and wear-resistant coatings for current-and future-generation aircraft engines. UES provided on site support, abstract booklets and made all arrangements for the meeting. The number in attendance was 56 of which 46 gave presentations. UES provided travel and per diem for one advisor to attend.

Major Hugh De Long, Program Manager

- 3. The second program review entitled **Corrosion Review** was held on 30 January through 3 February 2000 at Hawk's Cay, Duck Key, FL. This program is designed to assist the Air Force meet their requirements beyond the year 2000, the establishment of a new coatings systems, with high performance, environmentally benign corrosion inhibitors in the conversion coating or primer is needed. There were 54 in attendance of which 34 were speakers. Travel and per diem was provided by UES for two advisors to attend. UES provided abstract booklets, onsite support and handled all arrangements for this review. *Major Paul Trulove, Program Manager*
- 4. The fourth program review entitled 4th Annual Review of AFOSR MURI "Nanoscale Devices and Novel Engineered Materials" was held on 4 February 2000 at Hawk's Cay, Duck Key, FL. Twelve speakers gave presentations in this area of research. UES provided on-site support and all arrangements for this review.

 Major Paul Trulove, Program Manager
- 5. The AFOSR/ONR Electrochemistry Science & Technology Review was held 14-16 February 2000 at the Radisson Hotel, Alexandria VA. The electrochemistry program involves molten salt systems for compact power sources and new alloy systems for a variety of Air Force systems. Specifically, to understand structure property relationships for future materials needs. thin magnetic and alloy film growth kinetics and mechanisms at the surface to understand structure property relationships for future material needs. There were 55 in attendance of which 46 were speakers. UES provided on-site support and handled all arrangements for this review. Travel and per diem was provided to one advisior to attend this program review. Major Paul Trulove, Program Manager

C. Workshops

1. The **Human Effects Workshop** was held in Mesa, Arizona on 26-27 April 1999. Thirteen advisors made a site visit to the Williams Gateway Airport on 26 April and then convened at the Arizona Golf Resort and Conference Center on 27 April 2000. UES provided travel and per diem for 12 advisors to attend.

Dr. Willard Larkin, Program Manager

C. Workshops - continued

2. On 27-28 May 1999 a workshop on **Polymer Composites** was held at the Hyatt Regency, Long Beach, CA. There were 17 in attendance. UES provided meeting space and audiovisual equipment. Seven advisors were provided travel and per diem to attend the workshop by UES.

Dr. Charles Lee, Program Manager

3. The Defense Advanced Research Projects Agency (DARPA) held a workshop on their HEDM program entitled **1999 DARPA HEDM Workshop**. The workshop was held at the Holiday Inn Cocoa Beach, Cocoa Beach, FL, 11 June 1999. UES provided on-site support and meeting site.

Dr. Michael R. Berman, Program Manager

D. Scientific Panel Meeting

The Molecular Dynamics/Theoretical Chemistry Panel Meeting was held 3 June 1999 at the Embassy Suites Alexandria, Alexandria, VA. UES secured 31 reviewers for the 11 proposals reviewed. Abstract booklets, meeting space and audio visual equipment rental was arranged by UES. Six panel members were provided with honorarium, per diem and travel.

E. Advisors

Melissa M. Mallis, Chemistry and Life Sciences Directorate, Air Force Office of Scientific Research, Arlington, VA, 31 March 1999.

Michael Jaffee, I. C. Khoo, **AFOSR MURI Meeting**, California Institute of Technology, Pasadena, CA, 8-9 April 1999

John M. Carroll, Terry Connolly, Colin G. Drury, Daniel R. Ilgen, Richard J. Jagacinski, Bonnie Elizabeth John, Kurt Kraiger, Willard Larkin, William S. Marras, Raja Parasuraman, Karlene Roberts, Kim J. Vicente, Greg L. Zacharias, **Human Effects Workshop**, Mesa, Arizona, 26-27 April 1999.

Willard Larkin, **PRET Workshop on Biomathematical Models**, Harvard University and Endicott Conference Center, Dedham, MA, 19-21 May 1999

Peter Achermann, Torbjorn Akerstedt, Alexander Borbely, David F. Dinges and Dale M.Edgar, **Workshop on Biomathematical Models**, 19-21 May 1999

Judy Chen, John C. Halpin, Brian S. Hayes, John L. Kardos, Madhu S. Madhukar, Karl Nelson and James Seferis, **Polymer Composites Workshop**, Hyatt Regency, Long Beach, CA, 24-28 May 1999

James V. Coe, Jimmie D. Doll, Bruce C. Garrett, Paul L. Houston, James M. Lisy and James J. Valentini, **Molecular Dynamic/Theoretical Chemistry Panel Meeting**, Embassy Suites, Arlington, VA, 3 June 1999

E. Advisors - continued

Harold Shechter, **High Energy Density Matter Program Review**, Holiday Inn Cocoa Beach, Cocoa Beach, FL, 8-11 June 99

Jorn Larsen-Basse, Steven T. Patton, Andrey A. Voevodin, **Tribology Program Review**, Cheeca Lodge, Islamorada, FL, 14-18 June 1999

Willard Larkin, Conference on Simulation-Based Human Performance, University of Georgia, Athens, GA, 24-27 June 1999

Willard Larkin, US Air Force Academy and research laboratories in Colorado, Colorado Springs, CO, 2-3 August 1999

Nancy Cooke, Randall Engle, John Jonides, Patrick Kyllonen, **AFOSR MURI Review Meeting**, George Mason University, Fairfax, VA, 28-29 October 1999

Priya Vashishta, panel meeting on **Applying Molecular & Materials Modeling**, Princeton, NJ, 16-20 January 2000 and Albuquerque, NM, 20-22 January 2000

Keiji Morokuma, panel meeting on Applying Molecular & Materials Modeling, Princeton, NJ, 16-20 January 2000

Hugh De Long and Patrick Hagans, **2000 Corrosion Review**, Hawk's Cay, Duck Key, FL, 30 January-4 February 2000

Robert Mantz, AFOSR/ONR Electrochemistry Science & Technology Review, Radisson Hotel, Alexandria, VA, 14-16 February 2000

F. Miscellaneous

The Proceedings of the High Energy Density Matter (HEDM) Contractors Conference, November 1999 was compiled, published and distributed to all attendees during this reporting period.

SUMMARY

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Dr. Mike Livingston, Program Manager; Judith M. Flory, Program Administrator; and Ms. Ann Corbitt, Program Assistant. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

LIST OF APPENDICES

- A. Breakdown of Research Proposals by Program Manager
- B. Program for AFOSR Polymer Composites Workshop, Hyatt Regency, Long Beach, CA, 28 May 1999
- C. Summary of Review, AFOSR Molecular Dynamics/Theoretical Chemistry Review Panel Meeting, Embassy Suites Alexandria, Alexandria, VA, 3 June 1999.
- D. 1999 High Energy Density Matter Contractor's Meeting, Holiday Inn Oceanfront Resort, Cocoa Beach, FL, 8-10 June 1999
- E. 1999 DARPA HEDM Workshop, Holiday Inn Oceanfront Resort, Cocoa Beach, FL, 11 June 1999
- F. AFOSR/ONR/NSF Tribology Program Review, Cheeca Lodge, Islamorada, FL, 14-18 June 1999
- G. 2000 AFOSR Corrosion Review, Hawk's Cay, Duck Key, FL,
 30 January -3 February 2000
- H. 4th Annual Review of AFOSR MURI, Hawk's Cay, Duck Key, FL, 4 February 2000
- I. AFOSR/ONR Electrochemistry Science & Technology Review, Radisson Hotel, Alexandria, VA, 14-16 February 2000
- J. Annual Report, Chemistry and Life Sciences Research Program, Contact No. F49620-95-C-0026, Period of Performance: 3/15/95 2/29/96
- K. Annual Report, Chemistry and Life Sciences Research Program, Contact No. F49620-95-C-0026, Period of Performance: 3/15/96 2/28/97
- L. Annual Report, Chemistry and Life Sciences Research Program, Contact No. F49620-95-C-0026, Period of Performance: 3/15/97 2/28/98
- M. Annual Report, Chemistry and Life Sciences Research Program, Contact No. F49620-95-C-0026, Period of Performance: 3/15/98 2/28/99

BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER

Program Manager	Number of Proposals	
Michael Berman	14	
Robert Cohn	1	
Hugh De Long	9	
Walter Kozumbo	4	
Willard Larkin	21	
Charles Lee	17	
Paul Trulove	1	

AGENDA

AFOSR Polymer Composites Workshop

28 May 1999

Hyatt Regency Long Beach Long Beach, CA

0800	Simulated Laminated Methodology for Environmental Cycling of Polymer Composites James C. Seferis, University of Washington
0835	The Durability Characterization of High Temperature Polymer Matrix - Carbon Fiber Composites for Future Aerospace Application Roger J. Morgan, Michigan State University
0910	Moisture Transport and Thermal Aging Damage Mechanisms in Polymer Matrix Composites Albert F. Yee, University of Michigan
0945	Break
1000	The Durability Characterization of High Temperature Polymer Matrix – Carbon Fiber Composites for Future Air Force Application Chuk L. Leung, PolyComp Technologies, Inc.
1035	Durability Characterization of High Temperature Polymer Matrix – Carbon Fiber Composites for Future Air Force Applications: Development of Constitutive Models that Include Physical and Chemical Aging J. M. Caruthers, Purdue University
1110	Service Environmental Durability of High Performance Polymers and Composites David Curliss, AFRL/MLBC, Wright-Patterson AFB
1145	Characterizing Physical Aging in Polymeric Composites C. T. Sun, Purdue University
1205	Lunch
1300	Characterization of Aging, Deformation and Failure of High-Temperature Polymer Matrix Composites Isaac M. Daniel, Northwestern University
1320	Lightweight Structural Materials Research at Prairie View A & M University Fast Center Paul O. Biney, Prairie View A & M University Fast Center
1355	Structural Foams of Improved Strength and Thermal Stability from Random-Coil and Rigid-Rod Polymers Seng C. Tan, Wright Materials Research Co., Jim Mark, University of Cincinnati
1430	Cure Cycle Optimization to Minimize Cure Induced Stresses Madhu S. Madhukar, The University of Tennessee
1505	Adjourn

SUMMARY OF REVIEWS AFOSR Molecular Dynamics/Theoretical Chemistry Review Panel Meeting

99-NL-080 Spectroscopy and Dynamics of Transient Energetic Species

-Robert Continetti, University of California, San Diego

James V. Coe, The Ohio State University (A/1)

Paul L. Houston, Cornell University (A/2)

Marsha I. Lester, University of Pennsylvania (A-/2)

James M. Lisy, University of Illinois at Urbana-Champaign (A+/2)

99-NL-084 Physical Chemistry of Energetic Nitrogen Compounds

-Robert Coombe, University of Denver

Paul L. Houston, Cornell University (A-/2)

James J. Valentini, Columbia University (C/2)

Ralph Weston, Brookhaven National Lab (A/3)

99-NL-085 Studies of Transition States and Cluster-Induced Reactivity via

Negative Ion Photoelectron Spectroscopy

-Daniel Neumark, University of California, Berkeley

Kit Bowen, Johns Hopkins University (A+/3)

James V. Coe, The Ohio State University (A+/1)

Paul L. Houston, Cornell University (A/2)

James J. Valentini, Columbia University (A/1)

99-NL-087 Cluster Ion Beam Studies of Fundamental Dynamics Related to Physical Deposition

-Scott L. Anderson, University of Utah

James V. Coe, The Ohio State University (B+/3)

James M. Lisy, University of Illinois at Urbana-Champaign (A-/4)

James J. Valentini, Columbia University (A/3)

Nicholas Winograd, Penn State University (A-/2)

99-NL-088 Understanding Failure of Thermal Barrier Coatings from First Principles

-Emily Carter, University of California, Los Angeles

Jimmie D. Doll, Brown University (A/2)

Bruce C. Garrett, Pacific Northwest National Laboratory (A/2)

Hannes Jonsson, University of Washington (B+/2)

Steven G. Louie, University of California at Berkeley (A/A-/1)

99-NL-090 Metal Solvation and Novel Metal-Ligand Interactions in Gas Phase Clusters

-Michael A. Duncan, University of Georgia

Peter B. Armentrout, University of Utah (B+/2)
Philip J. Brucat, University of Florida (A/1)
Paul L. Houston, Cornell University (A-/2)
James M. Lisy, University of Illinois at Urbana-Champaign (B+/1)

99-NL-094 State-Resolved Thermal/Hyperthermal Collisional Dynamics of Atmospheric Species

-David J. Nesbitt, University of Colorado

James V. Coe, The Ohio State University (A+/2) Paul L. Houston, Cornell University (A+/1) Arthur Suits, Lawrence Berkeley Laboratory (A/2) James J. Valentini, Columbia University (B+/1)

99-NL-097 Advanced Simulation of Metal Clusters

-Xiao-Qian Wang, Clark Atlanta University

Jimmie D. Doll, Brown University (Wavelet Theory A, Applications B/2)

Bruce C. Garrett, Pacific Northwest National Laboratory (B/2) Robert J. Harrison, Pacific Northwest National Laboratory (A/3) William A. Shelton, Oak Ridge National Laboratory (B+/2)

99-NL-098 Ultrafast Vibrational Spectroscopy of Energetic Materials and Energetic Mechanical Processes

-Dana Dlott, University of Illinois

Mark Berg, University of South Carolina (A+/2) Eric Borguet, University of Pittsburgh (A-/A-/2) James V. Coe, The Ohio State University (A/3.5) James J. Valentini, Columbia University (A-/2)

99-NL-101 Heterogeneous Catalysis and Metal/Metal-Oxide Interfaces: Interactions, Reactions and Size Effects

-Uzi Landman, Georgia Institute of Technology

Jimmie D. Doll, Brown University (A/2)
Bruce C. Garrett, Pacific Northwest National Laboratory (A/2)
Michael Klein, University of Pennsylvania (A/not available)
Steven G. Louie, University of California at Berkeley (A/1)

99-NL-109 Oxidation Processes on Aluminum and Rhodium

-Andrew M. Rappe, University of Pennsylvania

Jimmie D. Doll, Brown University (A/2)
Bruce C. Garrett, Pacific Northwest National Laboratory (A-/2)
Hannes Jonsson, University of Washington (A/2)
Steven G. Louie, University of California at Berkeley (A+/1)

99-NL-143 Quantum Simulations of Low Temperature High Energy Density Matter

-Gregory Voth, University of Utah

Jimmie D. Doll, Brown University (will bring review to meeting)

1999 High Energy Density Matter Contractor's Meeting Holiday Inn Cocoa Beach Oceanfront Resort Cocoa Beach, Florida 8-10 June 1999

Monday, 7 June 1999	
7:00 – 9:00 PM	Registration
Tuesday, 8 June 1999	
7:30 – 8:30 AM	Registration/Continental Breakfast
8:30 – 9:00 AM	Introductory Remarks Dr. Michael Berman, AFOSR
9:00 – 9:40 AM	AFRL HEDM Research: Perspectives, Progress, and Directions Dr. Jeffrey A. Sheehy, AFRL, Edwards AFB
9:40 – 10:20 AM	Cryosolid Propellants—The Last "Revolutionary" HEDM Concept Dr. Mario E. Fajardo, AFRL, Edwards AFB
10:20 – 10:50 AM	Break
10:50 – 11:30 AM	The Solvation of Light Metal Atoms in Liquid Helium Droplets Dr. Giacinto Scoles, Princeton University
11:30 AM – 12:10 PM	Superfluidity on Molecular Scales, in Real Time Dr. Vartkess Ara Apkarian, University of California, Irvine
12:10 – 2:00 PM	Lunch
2:00 – 2:40 PM	Fundamental Insights from HEDM Studies Dr. David R. Yarkony, Johns Hopkins University
2:40 – 3:20 PM	Spectral Theory of The Chemical Bond: General Formalism for Atomic Aggregates Dr. Peter W. Langhoff, AFRL, Edwards AFB
3:20 – 3:50 PM	Break

Tuesday, 8 June 1999 (Cont'd)

3:50 – 4:30 PM	Spectroscopic Characterization of Non-bonding Interactions of the Aluminum Atom Dr. Paul J. Dagdigian, Johns Hopkins University
4:30 – 5:10 PM	Adiabatic and Approximate Diabatic Potential Energy Surfaces for The Weakly-Bound Al-H ₂ Complex Dr. Millard H. Alexander, University of Maryland
7:30 – 9:30 PM	Propulsion for Microsatellites Moderator, Dr. Patrick Carrick, AFRL, Edwards AFB Air Force Microsatellite Propulsion Systems Dr. Ronald Spores, AFRL, Edwards AFB Scaling Issues and Design Considerations for Chemical Micropropulsion Systems Dr. Andrew D. Ketsdever, AFRL, Edwards AFB High Performance Chemical Propulsion for Satellite Applications Dr. Tom W. Hawkins, AFRL, Edwards AFB

Wednesday, 9 June 1999

7:30 – 8:30 AM	Registration/Continental Breakfast
8:30 – 9:10 AM	Bicyclopropylidene and 1,5-Hexadiyne from Bench Scale to Pilot Scale: Problems and Solutions Dr. Suresh C. Suri, AFRL, Edwards AFB
9:10 – 9:50 AM	New Synthetic Methodologies for Geminal Polynitroalkanes and The Chemistry of The New HEDM Family of Diazenium diolates Dr. D. Scott Bohle, University of Wyoming
9:50 – 10:30 AM	New Energetics Technology Dr. Robert Schmitt, SRI International
10:30 – 11:00 AM	Break
11:00 – 11:40 AM	New Energetic Salts for Monopropellant Candidates Dr. Greg Drake, AFRL, Edwards AFB
11:40 AM – 12:20 PM	Development of Advanced Solid Rocket Propellants Using New Energetic Ingredients Dr. Michael A. Dewey, Thiokol Propulsion

Wednesday, 9 June 1999 (Cont'd)

12:20 – 2:00 PM	Lunch
2:00 – 2:40 PM	Theory and Synthesis of New High Energy Density Materials Dr. Karl O. Christe, AFRL, Edwards AFB
2:40 – 3:20 PM	N ₂ O Dimers, Trimers and Tetramers: A New Class of Potential HEDMS? Dr. Rodney J. Bartlett, University of Florida
3:20 – 3:50 PM	Break
3:50 – 4:30 PM	Study of High Energy Species Enabled by Scalable Computing Dr. Mark S. Gordon, Iowa State University
4:30 – 5:10 PM	Synthesis of High-Energy High-Nitrogen Heterocycles Dr. Harold Shechter, The Ohio State University
7:30 – 9:30 PM	Poster Session
Thursday, 10 June 1999	
Thursday, 10 June 1999 7:00 – 8:00 AM	Registration/Continental Breakfast
•	Registration/Continental Breakfast Electronic Structure Calculations for Ions in Solution: Non-Empirical Models Dr. Chao-Ping Hsu, University of California at Berkeley
7:00 – 8:00 AM	Electronic Structure Calculations for Ions in Solution: Non-Empirical Models
7:00 – 8:00 AM 8:00 – 8:40 AM	Electronic Structure Calculations for Ions in Solution: Non-Empirical Models Dr. Chao-Ping Hsu, University of California at Berkeley Laser Diagnostics for Aerosol Combustion Chemistry
7:00 – 8:00 AM 8:00 – 8:40 AM 8:40 – 9:20 AM	Electronic Structure Calculations for Ions in Solution: Non-Empirical Models Dr. Chao-Ping Hsu, University of California at Berkeley Laser Diagnostics for Aerosol Combustion Chemistry Dr. Roger E. Miller, University of North Carolina Nonadiabatic Dynamics of Photoexcited Reactions and Solvation Effects for Fundamental Organic Reactions

Thursday, 10 June 1999 (Cont'd)

11:10 – 11:50 AM	Ultrafast Dynamics of Energetic Materials: Towards an Understanding of Impact Sensitivity Dr. Dana D. Dlott, University of Illinois
11:50 AM - 12:30 PM	Atomic Propellants for Aerospace Propulsion Systems: Solid Hydrogen Experiments and Vehicle Analyses Dr. Bryan Palaszewski, NASA John H. Glenn Research Center
12:30 – 12:45 PM	Closing Remarks, adjourn Dr. Michael Berman, AFOSR
1:30 – 7:00 PM	Lunch and tours at Kennedy Space Center

1999 DARPA HEDM **WORKSHOP AGENDA**

11 June 1999 Date:

Holiday Inn Oceanfront Resort Cocoa Beach, Florida Location:

Friday 11 June

8:00 - 8:20 a.m.	Dr. Morrish, DARPA Welcome
8:20 - 8:30	Dr. Berman, AFOSR Comments
8:30 - 9:00	Dr. Bartlett, University of Florida
9:00 - 9:30	Dr. Christe, Dr. Wilson and Dr. Sheehy, Air Force Research Lab Edwards
9:30 - 10:00	Dr. Karle, NRL
10:00 - 10:30	Break
10:30 - 11:00	Dr. Oestmark, Swedish FOA
11:00 - 11:30	Dr. Lorenzana, Lawrence Livermore Nat'l Lab
11:30 - 12:00	Dr. Russled, Naval Research Lab
12:00 - 1:00	Lunch
1:00 - 1:30	Dr. Radziszewski, Colorado School of Mines
1:30 - 2:00	Dr. Funk, Los Alamos National Lab
2:00 - 2:30	Open Speaker
2:30 - 3:30	Group Discussion, Dr. Ladouceur, Moderator
3:30 - 3:45	Dr. Morrish, Concluding Remarks
3:45	Adjourn

AFOSR/ONR/NSF Tribology Program Review Cheeca Lodge Islamorada, Florida 14-18 June 1999

Sunday, 13 June 1999

1800-2100 Registration/Reception

Monday, 14 June 1999

0730	Registration/Continental Breakfast
0800	Progress in the Surface Science of Vapor Phase Lubrication and Frictional Properties of Single Crystalline Surfaces Andrew J. Gellman, Carnegie Mellon University
0830	Predicting Friction for a Vapor Lubricant Film in a Concentrated Contact Based on Principles of Solid Mechanics Nelson H. Forster, Air Force Research Laboratory
0900	Vapor Phase Lubricants: Nanometer-Scale Mechanisms and Applications to Sub-Micron and Rotating Machinery Jacqueline Krim, North Carolina State University
0930	Reactivity of Phosphate Esters with Various Substrates <u>Costandy S. Saba</u> and David W. Johnson, University of Dayton Research Institute Nelson H. Forster, Air Force Research Laboratory
1000	Break
1030	Wear Behavior of Irradiated Linear Polymer in Multi-Directional Sliding Contacts Thierry A. Blanchet and Brian R. Burroughs, Rensselaer Polytechnic Institute
1100	Modeling the Behavior of Polymer Nanocomposites Under Shear Anna C. Balazs, University of Pittsburgh
1130	Lunch
1300	New Materials for Controlling Friction and Wear in Extreme Environments: Synthesis, Tribochemistry, and Friction Mechanisms <u>Jeffrey S. Zabinski</u> , K. Strong, and P. J. John, Air Force Research Laboratory

Monday, 14 June 1999 (Cont'd)

1330	Real-Time Raman Tribometry: Friction, Wear and Third-Body Processes en Route to Failure S. D. Dvorak, <u>Kathryn J. Wahl</u> , and I. L. Singer, U. S. Naval Research Laboratory
1400	X-Ray SFA Studies of Molecular Organization and Surface Deformations During Lubricated Sliding <u>Jacob Israelachvili</u> , Yuval Golan, Ana Martin, Youli Li and Cyrus Safinya, <u>University of California at Santa Barbara</u>
1430	Computer Simulation of Sliding Hydroxylated Alumina Surfaces David Mann, Wayne State University

Tuesday, 15 June 1999

Tucsuay, 15	June 1777
0700	Registration/Continental Breakfast
0800	First-Principles Predictions of Cleavage Energies and Fracture Toughnesses, and Simulations of Crack Propagation in Polycrystalline Diamond <u>Donald W. Brenner</u> and Olga A. Shenderova, North Carolina State University
0830	Wide Temperature Range Gas-Phase Lubrication of Polished Polycrystalling Diamond Films with Molecular Oxygen for Extreme Environment MEMS Applications Michael N. Gardos, Raytheon Systems Company
0900	Tribology of MEMS Materials and Devices in Extreme Environments Steven T. Patton, and J. S. Zabinski, Air Force Research Laboratory
0930	Molecular Dynamics Investigations of the Tribology Hydrocarbon Containing Systems Judith A. Harrison, United States Naval Academy
1000	Break
1030	Tribological Behavior of Polished Polycrystalline α-SiC in Vacuum and 0.2 Torr/3.4 Torr Partial Pressures of Oxygen for Extreme Environment MEMS Applications Michael N. Gardos, Raytheon Systems Company
1100	Development and Application of Ultrahigh Resolution, Chemically-Sensitive Carbon Nanotube Probes for Surface Studies Charles M. Lieber, Harvard University

Tuesday, 15 June 1999 (Cont'd)

1130	Lunch
1300	Applications of a Non-Contacting Kelvin Probe During Sliding David A. Rigney, The Ohio State University
1330	Kelvin Probe Measurements Applied to Bearing Diagnostics <u>Steven Danyluk</u> and YeYuan Yang, Georgia Institute of Technology
1400	Integrated Diagnostics Richard S. Cowan, Georgia Institute of Technology
1430	Tribochemical Diagnostics: Optical Instrumentation and Molecular Modeling Dor Ben-Amotz, Purdue University

Wednesday, 16 June 1999

0700	Registration/Continental Breakfast			
0800	The Surface Chemistry and Tribology of Metal Carbides and Nitrides <u>Scott S. Perry</u> , University of Houston, Steve Didziulis, The Aerospace Corporation			
0830	Enhanced Tribological Properties of TiN/CN _x Multilayer Coatings with an Equiaxed Microstructure Dmitry Epstein, Igor Polonsky, Leon M. Keer, Michael Graham, Monica de Mesquita Lacerda, Yu-Hsia Chen and Yip-Wah Chung, Northwestern University			
0900	In-Situ Studies of the Nucleation and Growth of Cubic Boron Nitride E. Bengu and Laurence D. Marks, Northwestern University			
0930	Tribological Performance and Initial Finite Element Modeling of Reactively Sputtered Single and Multi-layer Chromium Nitride Thin Films Suzanne L. Rohde, University of Nebraska			
1000	Break			
1030	Formation, Characterization, and Tribological Testing of Carbon Coatings on Silicon Carbide Produced in Chlorine Containing Gases at High Temperature D. A. Ersoy, <u>Michael J. McNallan</u> and Y. G. Gogotsi, University of Illinois at Chicago			

Wednesday, 16 June 1999 (Cont'd)

1100	Synthesis, Modeling and Tribological Characterization of Functionally Graded Coatings <u>Sanjay Sampath</u> , L. Prchlik, J. Gutlebar and T. Nakamura, State University of New York
1130	Lunch
1300	Sol-Gel Derived, Nanostructured Oxide Lubricant Coatings <u>Douglas J. Taylor</u> , Stuart T. Schwab, Patrick F. Fleig, TLP, Incorporated Richard A. Page, Southwest Research Institute
1330	Surface Micromapping and Self-Assembling Nanocomposite Molecular Lubricants Vladimir V. Tsukruk, Iowa State University
1400	Characterization and Wear Mechanisms of Carbide/Carbon/Dichalcogenide Nanocomposites for Aerospace Tribology <u>Andrey A. Voevodin</u> and J. S. Zabinski, Air Force Research Laboratory
1430	Nanotribological Studies of Bulk Ceramic Materials, Multilayered Thin Films, and Liquid Lubricant Films Bharat Bhushan, (Sriram Sundararajan presenting), The Ohio State University

Thursday, 17 June 1999

0700	Registration/Continental Breakfast
0800	Efficient Parallel Algorithms for Molecular Dynamics Simulations Using Variable Charge Transfer Electrostatic Potentials John W. Mintmire, U. S. Naval Research Laboratory
0830	Robust Variational Fitting and Integral Factorization: Variational Divide and Conquer Density-Functional Theory Brett I. Dunlap, Naval Research Laboratory
0900	Chemical-Mechanical Polishing Aided by Electrical Fields <u>Steven Danyluk</u> , Georgia Institute of Technology, Dae Soon Lim, Korea University
0930	Tribochemical Polishing of Silicon Nitride and Carbide <u>Trangott E. Fischer</u> , V. Muratov and Z. Zhu, Stevens Institute of Technology
1000	Break

Thursday, 17 June 1999 (Cont'd)

1030	Consequences of Simultaneous Mechanical and Chemical Stimuli at Tribological and Adhesive Interfaces Tom Dickinson, Washington State University
1100	Ruby Coatings for Tribological Systems Ursula J. Gibson, Dartmouth College
1130	Lunch
1300	Correlation Between Macroscopic Forces and Molecular Orientation: A Study of Ultrathin Organic Layers by Second Harmonic Generation (SHG) F. Eisert, A. Legant, M. Gurka, Manfred Buck, M. Grunze, Lehrstuhl für Angewandte Physikalische Chemie
1330	Vibration Characteristics of PZT Glide Heads Jin-Hui Ouyang and <u>I. Y. (Steve) Shen</u> , University of Washington, Alex Yl. Tasay, Castlewood Systems, Inc.
1400	Electrostatic Monitoring of Wear in Oil Lubricated Contacts Robert J. K. Wood, University of Southampton
1430	Investigation of Multiphase Nano-Structured Carbide Coatings for Rolling Contact Applications James E. Krzanowski, University of New Hampshire

Friday, 18 June 1999

0700	Registration/Continental Breakfast
0800	Analysis of Lip Seal Behavior Using A Mixed Soft Elastohydrodynamic Lubrication Model Fanghui Shi and Richard F. Salant, Georgia Institute of Technology
0830	Friction Study of Carbon Nanotubes <u>David T. Shaw</u> and Yan Chen, SUNY at Buffalo
0900	Soft Configuration Model for Wearless Sliding Friction <u>Alexander L. Burin</u> , Alexander Z. Patashinskii and Mark A. Ratner, Northwestern University
0930	An Investigation of Certain Dynamic Instabilities in Dry Sliding George G. Adams, Northeastern University

Friday, 18 June 1999 (Cont'd)

1000	Break
1030	Exploration of Tribological Coatings for MEMS Devices Gouri Radhakrishnan, The Aerospace Corporation
1100	Topics in Tribology of Manufacturing Operations Steven R. Schmid, University of Notre Dame
1130	Thermal-Tribological Designs and Studies of Tribological Contacts Qian (Jane) Wang, Northwestern University

2000 AFOSR Corrosion Review Hawk's Cay Resort Duck Key, FL

30 January – 3 February 2000

Sunday, 30 January 2000			
1800 – 2000	Registration/Reception		
Monday, 31	January 2000		
0730 - 0800	Registration/Continental Breakfast		
0800 - 0810	Welcoming and Introduction P. Trulove, Air Force Office of Scientific Research		
0810 - 0820	Coatings and Corrosion Protection Task – Overview M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH		
0820 - 0845	Novel Surface Preparation and Treatment Studies <u>M.S. Donley</u> , A.J. Vreugdenhil ¹ , V.N. Balbyshev ² , M. Khobaib ¹ , N.V. Voevodin ¹ , G.A. Pacinda ¹ , R.H. Parkhill, L.A. Kasten ¹ , and J.T. Grant ¹ , Air Force Research Laboratory, Wright-Patterson AFB, OH, ¹ University of Dayton Research Institute, ² Universal Technology Corporation,		
0845 – 0905	Characterization of a Novel Silicon Sol-Gel Chemistry for Al2024T3 Protection <u>A.J. Vreugdenhil</u> , V.N. Balbyshev, and M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH		
0905 - 0925	Electrochemical Investigation of a Silicon Sol-Gel Treatment of Al 2024-T3 <u>V.N. Balbyshev</u> and M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH		
0925 – 0950	Organic Corrosion Inhibitors for Al 2024-T3 M. Khobaib and M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH		
0950 - 1000	Coatings and Corrosion Protection Task – Summary M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH		
1000 – 1015	Break		
1015 – 1045	Measurement of Localized Corrosion Propagation Rates in Al and Al Alloys G.S. Frankel, Fontana Corrosion Center, The Ohio State University, Columbus, OH		
1045 – 1115	Oxidation and Corrosion Passivation of Aluminum Surfaces		

J.T. Yates, University of Pittsburgh, Pittsburgh, PA

Monday, 31 January 2000 (Cont'd)

- 1115 1145 Selective Chemical Etching of Cu-Rich and Fe-Rich Inclusions from the Surface of Aluminum AA 2024-T3 Alloy

 D. Buttry, Department of Chemistry, University of Wyoming, Laramie, WY
- 1145 1315 Lunch
- 1315 1345 Nondestructive Characterization of Pitting Corrosion Damage S.I. Rokhlin, The Ohio State University, Columbus, OH
- 1345 1415 The Role of Coating and Substrate Heterogeneities in the Long Term Performance of Painted Aluminum Alloys: Local Detection and Mapping of Coating Defects

 S.R. Taylor and A.M. Mierisch, Center for Electrochemical Science and Engineering Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA
- 1415 1445 The Role(s) of Substrate Alloy Heterogeneity in the Corrosion of Painted Aluminum Alloys

 J.R. Scully and G.O. Ilevbare, Center for Electrochemical Science and Engineering, Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA
- 1445 1515 Influence of the Bulk Solution Composition on the Blister Formation of AA2024
 O. Schneider and R.G. Kelly, Center for Electrochemical Science and Engineering
 Department of Materials Science and Engineering University of Virginia,
 Charlottesville, VA

Tuesday, 1 February 2000

- 0730 0800 Continental Breakfast
- 0800 0840 The Development of an Environmentally Compliant Corrosion Resistant and Electrically Conductive Corrosion Coating for Aluminum

 S.R. Taylor, R.B. Leggat, and E. Pehovaz, University of Virginia, R.G. Buchheit, W. Zhang, M. Babu, A. Sehgal, L. Flores, and V. Laget, The Ohio State University T. Gaddy, M. Josefowicz, and P. Patel, Clariant Corporation
- 0840 0905 Self-Healing in Chromate-Free Conversion Coatings

 <u>R.G. Buchheit</u>, S.G. Mamidipally, H. Guan, P. Schmutz, V.N. Laget,
 The Ohio State University, Columbus, OH
- 0905 0925 Critical Factors for the Transition from Chromate to Chromate-Free Corrosion Protection

 R.G. Buchheit¹, J.H. Beatty², M.S. Donley³, G.S. Frankel¹, H.L. Fraser¹, and R.L. McCreery¹, ¹ The Ohio State University, ²Army Research Laboratories, ³Air Force Research Laboratory
- 0925 0955 Development of Non-Chromated Aerospace Coatings for Military Aircraft

 J. Stoffer, University of Missouri-Rolla, Rolla, MO

Tuesday, 1 February 2000 (Cont'd)

0955 – 1010	Break			
1010 – 1040	Importance of Adhesion in Corrosion Protection of Aluminum Alloys H. Yasuda, University of Missouri-Columbia, Columbia, MO			
1040 – 1110	Trimethylsilane Plasma Coatings on IVD Aluminum J. Deffeyes, The Boeing Company, St. Louis, MO			
1110 – 1140	Environmentally Compliant Thermal Spray Coatings for Wear and Corrosion Control K. Legg, Rowan Technology Group, Libertyville, IL			
1140 - 1310	Lunch			
1310 – 1340	Advanced Corrosion Resistant Aircraft Coatings for Outer Mold Line Applications J.H. Osborne, The Boeing Company, Renton, Washington			
1340 – 1410	Sol-gel Coatings with Organic Corrosion Inhibitors <u>S.F. Cogan</u> , M.D. Gilbert, P.J. Marren, and J. Ehrlick, EIC Laboratories, Inc., Norwood, Massachusetts J.H. Osborne, D.I. Dull, The Boeing Company, Renton, Washington			
1410 –1440	Development of Hybrid Organic-Inorganic Coatings for Aircraft Aluminum Alloys E.T. Knobbe, Department of Chemistry and the Environmental Institute, Oklahoma State University, Stillwater, OK			
1440 – 1500	Electrochemical Impedance Spectroscopy Studies of a Double Strand Polyaniline Coating on Aluminum Alloys in Acidic Environments R. Racicot, US Air Force Academy, CO			
	"Discussion"			
Wednesday, 2 February 2000				
0730 - 0800	Continental Breakfast			
0800 – 0840	Mechanism of Al Alloy Corrosion and the Role of Chromate Inhibitors G.S. Frankel, C.R. Clayton, R.D. Granata, M.W. Kendig, H.S. Isaacs, R.L. McCreery, S. Smialowska, and M. Stratmann, The Ohio State University, Columbus, OH			
0840 – 0910	Structure and Dynamics of Chromate Films on Aluminum Aircraft Alloy Probes with Vibrational Spectroscopy R.L. McCreery, The Ohio State University, Columbus, OH			
0910 - 0920	Break			

Wednesday, 2 February 2000

Fargo, ND

0920 - 1000 Copper Redistribution during Corrosion and Pretreatment of Aluminum Alloy 2024 K. Sieradzki, N. Dimitroiv, C. Droneburg, J. Mann, and M. Vukmirovic, Arizona State University, Tempe, AZ High Resolution Analytical Microstructural Analysis of Corrosion Induced Changes in 1000 - 1030Al Alloy 2024 R. Carpenter, Arizona State University, Tempe, AZ 1030 - 1050 Redistribution of Cathodic Reaction Kinetics During Corrosion of AlCuMg Alloys T.J.R. Leclere and R.C. Newman, UMIST, Corrosion and Protection Centre. Manchester, UK 1050 - 1100 Break 1100 – 1120 Current Corrosion Research Activities at the Army Research Lab P.F. Buckley, Army Research Laboratory, Aberdeen Proving Ground, MD 1120 - 1220 Open Discussion - Future Directions in Air Force Corrosion Research D. Peeler and P. Trulove **OPEN AFTERNOON** Thursday, 3 February 2000 0730 – 0800 Continental Breakfast 0800 - 0830 Electrochemical, Appearance, and Contact Angle, Measurements of Aircraft Coating Systems in Combined OUV/Prohesion Exposure G.P. Bierwagen and J. Li, North Dakota State University, Fargo, ND 0830 - 0850 Characterization of Corrosion in Coated Metal System by Electrochemical Methods G.P. Bierwagen and M. Zidoune, North Dakota State University, Fargo, ND Spectroscopic Examination of Air Force Coatings Systems During Combined 0850 - 0910**OUV/Prohesion Exposure** A. Vreugdenhil, C. Vang, and G.P. Bierwagen, North Dakota State University, Fargo, ND AFM and SEM Studies on Aircraft Coatings under Accelerated Weathering Exposure 0910 - 0930X. Yang, D. Tallman, and G.P. Bierwagen, North Dakota State University, Fargo, ND 0930 - 0945 Break 0945 – 1005 Scanning Vibrating Electrode Studies of Chromated Epoxy Primer and Poly(3-Octyl Pyrrole) Coatings on Steel and Aluminum G.P. Bierwagen, D. Tallman, J. He, and V. Johnston, North Dakota State University,

Thursday, 3 February 2000 (Cont'd)

1005 – 1025	Studies of Conducting Polymer Poly(3-OctylPyrrole) for Corrosion Protection V. Johnston and G.P. Bierwagen, North Dakota State University, Fargo, ND			
1025 – 1055	EIS/ENM Instrumentation Studies <u>D. Farden</u> and <u>G. Miramontes De Leon</u> , North Dakota State University, Fargo, NL			
1055 – 1105	In Situ Detection of Corrosion: Comparison of EIS and ENM Results from Different Experimental Electrode Configurations G. Miramontes, X. Wang, and G.P. Bierwagen, North Dakota State University, Fargo, ND			
1105 – 1125	New High Performance Polysiloxane Primers for Aluminum T.E. Ready, <u>P. Boudjouk</u> , S. Rohlik, V. Gelling, D. Tallman, G.P. Bierwagen, North Dakota State University, Fargo, ND			
1125 – 1300	Lunch			
1300 – 1320	Planned Studies on the Synthesis of Probe Molecules for Better Characterization of Coating Degradation M. Sibi, North Dakota State University, Fargo, ND			
1320 – 1340	Magnesium Powder Filled Ambient-Cure Epoxy Primers for Aluminum 2024 T-3 G.P. Bierwagen, North Dakota State University, Fargo, ND			
1340 – 1405	SVET Studies of Corrosion Initiation and Progression Under Coatings <u>M. Khobaib</u> , A. Buchanan and M. Donley, University of Dayton Research Institute, Dayton, OH and Air Force Research Laboratory, Wright-Patterson AFB, OH			
1405 – 1430	Implementation of a Hidden Corrosion Detection Assessment Methodology W. Hoppe, University of Dayton Research Institute, Dayton, OH			
1430 – 1445	A Look Back at the AF Blue Ribbon Panel M.S. Donley, Air Force Research Laboratory, Wright-Patterson AFB, OH			
1445 – 1545	Open Discussion – Future Directions in AF Paint and Coatings Research B. Ghim and P. Trulove			
1545	Closing Remarks P. Trulove			

Agenda

4th Annual Review of AFOSR MURI "Nanoscale Devices and Novel Engineered Materials" University of Florida

Monitor: Maj. Paul Trulove, Ph.D.

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February 4, 2000 Location: Hawk's Cay Resort, Marathon, FL

Location: Hawk's Cay	Resort, Marathon, FL
9:00-9:20 am	Welcome and Overview; Program Goals and Achievements S.J. Pearton (MSE/UF)
9:20-9:40 am	Mechanical Properties of Nanostructured Materials S.A. Syed Asif (NRL)
9:40-9:55 am	Magnetotransport – charge, frequency and noise properties A.F. Hebard (Physics/UF)
9:55-10:30 am	Physics of Length Scales in Magnetic and Superconducting Microstructures, I.K. Schuller (Physics/UCSD)
10:30-11:00 am	Coffee Break
11:00-11:20 am	Integration of Magnetic Nanoparticles with 2-D Electron Systems S. von Molnar (Physics/FSU)
11:20-11:40 am	Nanostructure Patterning and Transport Physics F. Sharifi (Physics/UF)
11:40-12:00 am	Ion Beam Deposited GMR Materials D. Temple and G.E. McGuire (MCNC)
12:00-1:30 pm	Lunch
1:30-1:50 pm	Dry Etching of Magnetic Multilayers, S.J. Pearton (MSE/UF)
1:50-2:05 pm	Integration of Magnetic Materials and Semiconductors F. Ren (Chem. Eng./UF)
2:05-2:20 pm	Deposition and Etching of Ferromagnetic Particles in a Non Magnetic Matrix, A.C. Kummel (Chem/UCSD)
2:20-2:35 pm	Pulsed Laser Deposition of CMR Oxides, R.K. Singh (MSE/UF)
2:35-3:00 pm	Theory and Modelling of GMR, S. Hershfield (Physics/UF)
3:00-3:15 pm	Summary and Accomplishments, S.J. Pearton
3:15-3:45 pm	Discussion (all)

AFOSR/ONR Electrochemistry Science & Technology Review Radisson Hotel Alexandria, VA

14 – 16 February 2000

Monday, 14 February 2000

12:00-1:00	Registration
1:00-1:25	Welcoming and Introduction R. Carlin, Office of Naval Research, Arlington, VA; P. Trulove, Air Force Office of Scientific Research, Arlington, VA
1:25–1:50	Nanotubule Membranes – Fundamentals and Applications in Electrochemical Energy and Stochastic Sensing C. Martin, University of Florida, Gainesville, FL
1:50-2:15	Aerogel-based Batteries: En route to a 3-D Nanoscopic Battery D. Rolison, Naval Research Laboratory, Washington, DC
2:15-2:40	Electrochemical Properties of Sol-Gel Derived Materials B. Dunn, UCLA, Los Angeles, CA
2:40-2:55	Break
2:55–3:20	Charge Transfer Systems of Molecular Dimensions R. Murray, University of North Carolina, Chapel Hill, NC
3:20–3:45	Dendritic- and Fractal-Based Nanotechnologies for Electrochemical Studies <u>G. Newkome</u> , T. J. Cho, A. Mishra, C. Moorefield, G. Baker; University of South Florida, Tampa, FL
3:45-4:10	Dendrimer-Encapsulated Metal Nanoparticles R. Crooks, Texas A&M University, College Station, TX
4:10–4:35	Extended Structures by Metal-Initiated Self-Assembly and Electrode Surface Structure and Composition Effects on Formic Acid Electrocatalysis H. Abruña, Cornell University, Ithaca, NY
4:35–5:00	Synthesis of Redox-Active and Porous Supramolecular Structures M. Ward, University of Minnesota, Minneapolis, MN
5:30	Reception

Tuesday, 15 February 2000

7:30-8:00	Continental Breakfast
8:30-8:55	Electron and Ion Transfer at Interfaces R. Marcus, California Institute of Technology, Pasadena, CA
8:55-9:20	Dip-Pen Nanolithography: A New Tool for Generating and Studying Soft Nanostructures C. Mirkin, Northwestern University, Evanston IL
9:20-9:45	Nanoscale Assembly of Components for Rechargeable Lithium Batteries <u>D. Sadoway</u> , <u>A. Mayes</u> , MIT, Cambridge, MA
9:45-10:10	Nanocomposite Polymer Electrolytes E. Giannelis, Cornell University, Ithaca, NY
10:10-10:25	Break
10:25–10:50	Ionically Conducting Channel L. Scanlon, AFRL/PRPB, Wright-Patterson AFB, OH
10:50–11:15	Lithiated Macrocycles in the Search for New Li-Ion Conductors <u>J. Arnold</u> , A. Gebauer, University of California, Berkeley, CA
11:15–11:40	NMR Studies of Ion Transport in Disordered Media S. Greenbaum, Hunter College of the City University of New York, New York, NY
11:40–12:05	Passivation Prevention Using Self-Assembled Molecular Layers at the LI/Solid Polymer Electrolyte Interface D. Teeters, The University of Tulsa, Tulsa, OK
12:05-1:30	Lunch
1:30–1:55	Combinatorial, Highly Automated and Rapid Approaches to Electrocatalyst Development D. Buttry, University of Wyoming, Laramie, WY
1:55–2:20	Surface Electrochemistry of Catalytic Reactions at Temperatures Ranging from Ambient to 80 °C C. Korzeniewski, Texas Tech University, Lubbock, TX
2:20–2:45	Development of Electrochemical Capacitor Technology for DOD Applications A. Apblett, Oklahoma State University, Stillwater, OK
2:45–3:10	Preparation and Characterization of Nano-structured Materials for Solid-State Electrochemical Applications M. Collinson, Kansas State University, Manhattan, KS
3:10-3:50	Break

Tuesday, 15 February 2000 (Cont'd)

3:50-4:10	Electrodeposition of Transition Metal-Aluminum Alloys from Chloroaluminate Molten Salts C. Hussey, University of Mississippi, University, MS
4:10–4:30	The Electrodeposition of Al-Nb Alloys from Chloroaluminate Electrolytes <u>G. Stafford</u> , National Institute of Standards and Technology, Gaithersburg, MD; G. Haarberg, Norwegian University of Science and Technology, Trondheim, Norway
4:30-4:55	Studies in Buffered Chloroaluminate Ionic Liquids R. Osteryoung, North Carolina State University, Raleigh, NC
4:55–5:15	Ionic Liquids as Supporting Electrolytes for Supercapacitors J. Stenger-Smith, Research and Technology Group, NAWCWPNS, China Lake, CA
5:15–5:40	Physical Properties of the Pristine and Lithiated Substituted-Imidazolium Molten Salt Electrolytes as Liquids and as Polymer Gel Composites H. De Long, U. S. Naval Academy, Annapolis, MD
Wednesday	, 16 February 2000
7:30-8:00	Continental Breakfast
8:30–8:55	Electrochemistry at Nanostructured Materials: The Scaling of Molecular Transport in Small Domains H. White, University of Utah, Salt Lake City, UT
8:55–9:20	Fundamentals of Charge Transfer at Nanocrystalline Electrode/Solution Interfaces J. Hupp, Northwestern University, Evanston, IL
9:20–9:45	Influence of High Interfacial Electric Fields on the Dielectric Properties and Ionization of Water E. Stuve, University of Washington, Seattle, WA
9:45–10:10	Ruthenium Cluster Modification of Platinum Surfaces: Its Application on the Preparation of Pt/Ru Catalyst for Methanol Oxidation C. Cabrera, University of Puerto Rico, San Juan, Puerto Rico
10:10-10:25	Break
10:25–10:50	Preparation and Characterization of Thermoresponsive Polymeric Gels: Studies with Electroactive Probes M. Ciszkowska, Brooklyn College, Brooklyn NY
10:5011:15	Properties of Fuel Cell and Battery Materials P. Stallworth, J. Fontanella, M. Wintersgill, C. Edmondson, U.S. Naval Academy, Annapolis, MD S. Greenbaum, Hunter College of the CUNY, New York, NY

Wednesday, 16 February 2000 (Cont'd)

11:15-11:40	Modeling of On-board Fuel Cell-Based Power System for Naval Ships R. White, University of South Carolina, Columbia, SC
11:40-12:05	Development of Novel Electrode Materials for Use in H2S-Containing Gases S. Wang, M. Liu, <u>J. Winnick</u> , Georgia Institute of Technology, Atlanta, GA
12:05-1:30	Lunch
1:30-1:55	Development of New Fast Proton Conducting Chalcogenide Glassy Electrolytes S. Martin, Iowa State University, Ames, IA
1:55-2:20	Magnesium-Solution Phase Semi-Fuel Cell System Utilizing a Palladium/ Iridium Catalytic Surface M. Medeiros, E. Dow, Naval Undersea Warfare Center, Newport, RI, R. Bessette, University of Massachusetts Dartmouth, North Dartmouth, MA
2:20-2:45	Study of Lithium Polymer Interface to Enhance Efficiency and Safety in Lithium/Water Batteries M. Urquidi-Macdonald, J. Cho, Pennsylvania State University, University Park, PA
2:45-3:10	Redox Cycling of Manganese on Metal Surfaces and its Consequences for Material Performance Z. Lewandowski, Montana State University, Bozeman, MT
3:10-3:50	Break
3:50-4:15	Thermal and Electrochemical Models for Batteries During High Rates of Discharge J. Van Zee, University of South Carolina, Columbia, SC
4:15-4:40	X-ray Absorption Spectroscopy and Electrochemical Studies of Novel Materials for Li-Ion Batteries A. Mansour, NSWC/CD, West Bethesda, MD
4:40-5:00	Conductive Polymer Moderated Reactive Metal Anodes W. Ferrando, CDNSWC, West Bethesda, MD
5:00	Closing Remarks/Adjourn

APPENDIX J

ANNUAL REPORT

CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM CONTRACT NO. F49620-95-C-0026

PERIOD OF PERFORMANCE: 3/1/95 - 2/29/96

Prepared For:

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH CHEMISTRY AND LIFE SCIENCES DIRECTORATE

Dr. Genevieve Haddad, Program Manager

Presented By:

UES, Inc. 4401 Dayton-Xenia Road Dayton, OH 45432-1894

INTRODUCTION

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology, Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The first year core effort included: 132 Proposals that were reviewed; 2 Program/Contractor Reviews; 3 Workshops and 3 Scientific Panel Meetings.

A. Evaluations of Individual Research Proposals

UES sent out 132 proposals to 391 evaluators during the performance period of 1 March 1995 through 29 February 1996.

UES has been providing to the Directorate of Chemistry and Life Sciences a Summary of Proposals Under Review (SPUR) report on a biweekly basis. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the Program Managers to have a current listing of all proposal activity.

B. Contractor/Program Reviews

A total of 2 program reviews were held during this first contract year.

1. The first program review entitled **Predictive Toxicology** was held 31 May through 1 June 1995 at the Holiday Inn I-675 Conference Center, Fairborn, OH. The purpose of this meeting was to review basic research in toxicology which is supported by or of interest to the AFOSR program in Predictive Toxicology. There were 47 in attendance of which 26 were speakers that gave presentations discussing the primary objectives, results and conclusions of past research, emphasizing major accomplishments, and indicating new directions and areas of future research. The purpose of the review was to strive to achieve several goals; to inform each

research, emphasizing major accomplishments, and indicating new directions and areas of future research. The purpose of the review was to strive to achieve several goals; to inform each participant of other work being conducted under the AFOSR Toxicology Program; to exchange scientific information; to foster collaboration; and to generate new ideas. In addition, AFOSR acquired information that will facilitate technology transfers, Air Force justification of research efforts and decision-making with respect to programmatic organization.

Dr. Walter Kozumbo, Program Manger

2. The second program review entitled Nonlinear Optical Polymers Contractors Review Meeting was held on 26-28 February 1996 at the Holiday Inn I-675 Conference Center, Fairborn, OH. The purpose of this meeting was to coordinate Air Force sponsored research in this area and to promote transitions of research results to Air Force laboratories. The meeting included presentations by Air Force scientists describing potential applications for this class of materials and the desirable parameter spaces and other secondary properties necessary for these applications. Also, the Air Force applications that can potentially use nonlinear polymers and organic materials were included in this program review. The number in attendance was 104 of which 52 gave presentations.

Dr. Charles Lee, Program Manager

UES provided travel, per diem and honorarium for the 8 advisors who attended the Nonlinear Optical Polymers Contractors Review Meeting and then provided to AFOSR written overviews of the program reviews. UES also provided on site support, acquisition of meeting site and audio visual equipment.

C. Workshops

Three workshops were held during this first year's effort.

- 1. On 25 May 1995 a workshop on Environmental Effects on High Performance Polymers and Composites was held at the Holiday Inn I-675 Conference Center, Fairborn, OH. There were 22 in attendance. UES provided meeting space and audio visual equipment. Dr. Charles Lee, Program Manager
- 2. A workshop on Night Operations/Human Chronobiology was held at Bolling AFB, DC, 6-7 June 1995. UES provided travel, per diem, honorarium for the 8 advisors in attendance. Dr. Genevieve Haddad, Program Manager
- 3. A second workshop on **Night Operations/Human Chronobiology** was held on 3-5 January 1996 at Holloman AFB, NM. There were approximately 19 attendees. UES provided travel, per diem and honorarium to 8 advisors.

 Dr. Genevieve Haddad, Program Manager

D. Panel Meetings

- 1. A panel meeting was held on Atmospheric Effects of Rocket Exhaust at the College Inn Conference Center, University of Colorado, Boulder, CO on 28 September 1995. This panel meeting of six advisors was assembled to develop knowledge necessary to assess the impact of the exhaust from rocket motors on the atmospheric environment.
- 2. Hanscom AFB, MA hosted a panel meeting on the Review of Laboratory Tasks in the Molecular Dynamics Program, 2-3 November 1995. Five advisors participated in the review of the Air Force Phillips Laboratory's program in Molecular Dynamics at Hanscom AFB, MA.
- 3. A panel meeting was held on **Molecular Dynamics and Theoretical Chemistry** at the Marriott's Lincolnshire Resort, Lincolnshire, IL on 30 November 1995. Seven advisors reviewed proposals in the mentioned area.

UES provided abstract booklets for all three meetings as well as on site support for the Boulder CO and Chicago IL panel meetings. Meeting space, travel, per diem and honorarium were provided for the advisors for all three panel meetings.

E. Advisors

In addition to the advisors provided for meetings, Dr. Charles Czeisler was requested to give a seminar at The Aerospace Medical Association Meeting, 7-9 May 1995 in Annaheim, CA. Dr. Czeisler also gave an overview of the meeting for AFOSR. UES provided transportation and per diem for Dr. Czeisler.

SUMMARY

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Dr. Julien M. Christensen, Program Manager; Judith M. Flory, Program Administrator; and Ms. Betty Kerans, Program Assistant. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

LIST OF APPENDICES

Breakdown of Research Proposals by Program Manager

Program and Abstract Booklet for AFOSR Predictive Toxicology Program Review

Program for Air Force Nonlinear Optical Polymers Contractor's Review Meeting

BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER

PROGRAM MANAGER	NO OF PROPOSALS
Haddad	12
Tangney	13
Lee	24
Kozumbo	25
Kroll	11
Lewis	2
DeLong	17
Hedberg	3
Berman	22
Roach	3

AFOSR

PREDICTIVE TOXICOLOGY PROGRAM REVIEW

31 May - 1 June 1995

Holiday Inn Conference Center/I-675 Fairborn, Ohio



SPEAKERS

Basak, Subhash
Bernofsky, Carl
Dallas, Cham
Eurell, Thomas
Harris, David
Krishnan, Kannan
Miller, Clay
Myers, Charles
Pereira, Michael

Reo, Nicholas Risby, Terence Robledo, Raymond Siegel, Frank Smulson, Mark Stohs, Sidney Thomas, Russell Trosko, James Witzmann, Frank

AFOSR PREDICTIVE TOXICOLOGY PROGRAM REVIEW

Walter Kozumbo, Ph.D. Program Manager

SPONSORED:

for a

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH DIRECTORATE OF CHEMISTRY AND LIFE SCIENCES

UNDER CONTRACT #F49620-95-C-0026 UES, INC. 4401 Dayton-Xenia Road Dayton, OH 45432-1894



AFOSR PREDICTIVE TOXICOLOGY PROGRAM REVIEW Holiday Inn Conference Center/I-675 Fairborn, OH 31 MAY - 1 JUNE 1995

TUESDAY, 30 MAY 1995

1700-1830:

*Registration

1830-2030:

Evening Social at Holiday Inn

WEDNESDAY, 31 MAY 1995

0730-0830:

Registration/Continental Breakfast

INTRODUCTION

0830-0845:

AFOSR and Its Program in Predictive Toxicology

Dr. Walt Kozumbo, AFOSR, Bolling AFB

0845-0900:

Toxicology Program at Armstrong Laboratory/Tri-Service Toxicology

Dr. Jeff Fisher, Armstrong Laboratory, WPAFB

TOXICOLOGY AND PHARMACOKINETICS OF CHLORINATED SOLVENTS

(Dr. Miller as Moderator)

0900-0930:

Tools of Predictive Toxicology

Dr. Clay Miller, Armstrong Laboratory, WPAFB

0930-1000:

Carcinogenic Activity of Trichloroethylene and Chloroacetic Acids In Mouse Liver

Dr. Michael Pereira, Medical College of Ohio

1000-1015:

COFFEE BREAK

1015-1045:

Radical Intermediates of Halogenated Metabolites

Dr. Carl Bernofsky, Tulane University

1045-1115:

Interspecies Extrapolations of Halocarbon Tissue Toxicokinetics

Dr. Cham Dallas, University of Georgia

1115-1145:

An Interdisciplinary and Alternative Approach to Assess Carcinogenicity of

Chlorobenzenes

Mr. Russell Thomas/Dr. Raymond Yang, Colorado State University

1145-1300:

LUNCHEON at Holiday Inn

COMPUTATIONAL TOXICOLOGY AND MODELING OF TOXIC EFFECTS

(Dr. Fisher as Moderator)

1300-1330:

A Molecular Structure Based Modeling Framework for Predicting Pharmacokinetics of

Organic Chemicals

Dr. Kannan Krishnan, University of Montreal

1330-1400:

Use of Molecular Similarity Methods in the Risk Assessment of Chemicals:

A Study with Quadricyclane

Dr. Subhash Basak, University of Minnesota

MECHANISTICALLY BASED TOXICOLOGY

(Dr. Channel as Moderator)

1400-1430:

Mechanisms Associated with the Toxicity of Polyhalogenated Cyclic Hydrocarbons and

Heavy Metals

Dr. Sidney Stohs, Creighton University

1430-1445:

COFFEE BREAK

1445-1515:

Chromium Toxicity: Reductive Enzymes in Humans

Dr. Charles Myers, Medical College of Wisconsin

1515-1545:

Oxidative Stress, Gap Junctional Communication and Epigenetic Toxicology

Dr. James Trosko, Michigan State University

1545-1615:

Depletion of Nuclear Poly (ADP-ribose) Polymerase by Antisense RNA

Expression: Influences on DNA Repair and Replication, Genomic Stability, and Survival

of Cells to Genotoxic Agents

Dr. Mark Smulson, Georgetown University

1615:

ADJOURNMENT UNTIL TOMORROW MORNING

THURSDAY, 1 JUNE 1995

0730-0830:

BREAKFAST at Holiday Inn

BIOMARKERS AS PREDICTORS OF TOXICITY IN VITRO AND IN VIVO

(Dr. Channel as Moderator)

0830-0900:

Two-Dimensional Protein Pattern Recognition in Chemical Toxicity

Dr. Frank Witzmann, Indiana Univ.-Purdue Univ. at Columbus

0900-0930:

A Mechanistically Based, In Vitro Evaluation of Ocular Irritants

Dr. Thomas Eurell, University of Illinois at Urbana - Champaign

0930-1000:

NMR Spectroscopy as a Tool For Studies of Hepatotoxicity In Vivo

Dr. Nicholas Reo, Wright State University

1000-1030:

Biomarker Analysis of Human Breath for Early Prediction of Hepatotoxicity

Dr. Terence Risby, Johns Hopkins University

1030-1045: **COFFEE BREAK**

TOXICOLOGY OF JP-8 JET FUEL

(Dr. Fisher as Moderator)

1045-1115	The Chronic Effects of JP-8 Jet Fuel Exposure Mr. Ray Robledo/Dr. Mark Witten, University of Arizona
1115-1145:	Immunotoxicology of Exposure to JP-8 Jet Fuel and Halogenated Hydrocarbons Dr. David Harris, University of Arizona
1145-1215:	Detoxication Enzymes as Biomarkers of Toxin Exposure Dr. Frank Siegel/Dr. Steve Kornguth, University of Wisconsin
1215-1245:	OPEN DISCUSSION
1245-1300:	Concluding Remarks (Walt Kozumbo) and Toxicology Program suggestions by participants

^{*}Registered speakers and other active participants are kindly requested not to leave until the meeting has concluded.

MILLER Dr. Clay R. Miller

TOOLS OF PREDICTIVE TOXICOLOGY

Military operations require the use of numerous chemical compounds and materials. Many of these are unique to the military environment, with little information about their potential impact on the health of ground personnel or crew. Our work involves two lines of research. In the first, we have developed and validated mechanistically based assays to suggest the mechanism of toxic injury for the prototype high energy propellant, ammonium dinitramide (ADN). Using a novel reporter-gene construct linked to DNA promotion regulatory elements, we determined ADN's ability to alter cellular redox state. This suggested ADN would be an acute cytotoxicant with potential to interact with DNA. Electron paramagnetic resonance (EPR) studies demonstrated the radical products potentially produced from ADN biometabolism. The results suggested ADN to have a potential for mutagenicity. This potential was confirmed in a novel yeast translocation system and in a standard "Ames" battery. In a second line of research we have developed a pharmacodynamic (PD) model describing the mathematical dose-response for an acute biological event, lipid peroxidation. Ongoing studies using known positive compounds will be used to calibrate radical production as measured by EPR. Once validated, the PD model may serve as a template to predict similar biological effects of chemicals with no mechanistic toxicity data.

PEREIRA Dr. Michael A. Pereira

CARCINOGENIC ACTIVITY OF TRICHLOROETHYLENE AND CHLOROACETIC ACIDS IN MOUSE LIVER

Trichloroethylene is an industrial solvent and degreaser that has been extensively used by the U.S. Air Force and industry. Hazardous waste sites and groundwater have been found to be contaminated with trichloroethylene. In laboratory animals carcinogenic activity has been observed in mouse liver and lung and rat kidneys. Two major metabolites of trichloroethylene, dichloroacetic acid and trichloroacetic acid, have also been shown to be carcinogenic in mouse liver. However, both trichloroethylene and the two chloroacetic acids when assayed in genotoxic/mutagenic assays, have exerted either no activity or very weak activity. Therefore, tumor promotion has been proposed for the mechanism of trichloroethylene and its metabolites, especially in mouse liver. We have or are performing initiation-promotion bioassays for trichloroethylene and the two chloroacetic acids. Tumor promotion was observed for both dichloroacetic acid and trichloroacetic acid, however, both the dose response relationship and the characteristics of the lesions induced by the two chloroacetic acids differed. The dose response relationship for dichloroacetic acid exhibited a sharp increase between 6.67 and 20 mmol/liter, while trichloroacetic acid appeared to be linear over the range of concentrations evaluated. We are continuing to explore the dose response relationship for these chloroacetic acids and trichloroethylene, as well as to characterize the lesions and pathogenesis of the three compounds. One of our objectives is to determine whether the lesions and pathogenesis induced by dichloroacetic acid and/or trichloroacetic acid are consistent to those induced by trichloroethylene. Upon completion of these studies, we will supply a better understanding of the dose response relationship for these three compounds, as well as their mechanism of action and pathogenesis in mouse liver. This would improve and support the extrapolation of the carcinogenic results obtained in mouse liver to the estimation of the human health hazard of exposure to trichloroethylene.

BERNOFSKY Dr. Carl Bernofsky

RADICAL INTERMEDIATES OF HALOGENATED METABOLITES

1,1,2-Trichloroethylene (TCE) is an industrial solvent that is widely used for degreasing metals; it is also used for adhesives, paint stripping, dry cleaning, and in the manufacture of pharmaceuticals and textiles. Because of its widespread use and often improper disposal, TCE has become a common environmental contaminant at many worksites. It is also found in ground and surface waters near most large urban areas and at many landfill locations. Public exposure occurs through contaminated waters that are ultimately used for human consumption. TCE produces hepatocellular carcinomas and lung tumors in the mouse and renal tubular adenomas and testicular tumors in the rat. However, two TCE metabolites, trichloroacetic acid (TCA) and dichloroacetic acid (DCA), which are especially potent hepatocarcinogens in mice, have been implicated in the carcinogenicity of TCE. Although these haloacetic acid metabolites of TCE are capable of forming covalent adducts with DNA, the mechanism of adduct formation is unknown. By means of spin-trapping techniques, we will test the hypothesis that TCA and DCA are converted in the liver to reactive free radical intermediates that are responsible for forming these DNA adducts. Using mouse liver hepatocytes, we will examine the formation of free radicals in two ways: 1) directly, by means of electron paramagnetic resonance spectroscopy (EPR) of the trapped radicals, and 2) indirectly, through the use of a 14C-labeled spin trapping agent that will be converted to a stable derivative and quantitated by means of high-pressure liquid chromatography (HPLC). The rationale for the latter approach is based on recent evidence showing that viable cells have the ability to metabolize spin adducts to EPR-silent species, which could lead to a significant underestimate of radicals that have been trapped. We will also investigate the formation of DNA adducts by means of ³²P-postlabeling techniques, and we will determine the nature of these adducts by isolating the adducted DNA, digesting it with nucleases, and identifying the modified bases by means of HPLC and mass spectroscopy.

INTERSPECIES EXTRAPOLATIONS OF HALOCARBON TISSUE TOXICOKINETICS

The population of the U.S. is exposed to halocarabons occupationally and in the proximity of hazardous waste sites, as well as in ambient air and drinking water. Health risk assessments of such chemicals usually require extrapolating from the results of toxicity studies in animals to predict toxic effects in man. Interspecies extrapolations for halocarbons and other volatile organic compounds (VOCs) are necessary because of very limited human exposure data. Knowledge of the pharmacokinetics of a chemical provides important information that facilitates species to species extrapolations, and kinetic studies were therefore used in this project to enable the interspecies extrapolation of toxicokinetic data.

A series of experiments have been conducted to provide a pharmacokinetic data base for evaluating interspecies comparisons of the toxicokinetics of halocarbons, and for the formulation and validation of an accurate physiologically-based pharmacokinetic model. experimental design has involved giving equal does of halocarbons to rats, mice and dogs for pharmacokinetic and neurobehavioral toxicity comparisons. Perchloroethylene (PCE), tetrachloroethane (TET), trichloroethylene (TCE), and trichloroethane (TRI) have been employed as test chemicals, in order to evaluate the relative importance of the physiochemical property of volatility on the kinetics and toxicity of halocarbons. The respiratory elimination and systemic uptake of TCE, TRI and PCE has been measured in rats and compared to available human data. In order to determine the dose received in target organs and other tissues, serial samples of brain, liver, kidney, lung, heart, skeletal muscle, and adipose tissue have been taken and analyzed for halocarbon content after administration of PCE, TCE, TET, and TRI in rats, TRI in mice, and PCE and TET in dogs. In order to provide a toxicokinetic corollary with one of these target organs, the brain, a neurobehavioral operant testing system has been employed for monitoring the central nervous system effects of halocarbons. Neurobehavioral studies have been conducted following oral and inhalation exposure to PCE, and from inhalation exposure to TRI in rats and mice using the same exposure regimens as in the kinetic studies. There was a surprising similarity in exhaled breath levels for several halocarbons between rats in this project and with previously published human data. This occurred despite physiochemical differences in volatility that might have been expected to result in significant interspecies differences. Behavioral changes for equivalent exposure regimens in mice and rats did demonstrate significant interspecies differences. It was found that blood and brain deposition was related in a dose response fashion with neurobehavioral deficit, but the time course of kinetics and toxicity showed significant differences within species.

A major objective of the project has been to develop and validate a physiologically-based pharmacokinetic model for exposure to halocarbons. The direct measurement of halocarbon concentrations in exhaled breath and tissues provided an extensive data base that was highly useful in formulating and validating the model. The model has been scaled up from the rat to dog, and their ability to predict the time-course of respiratory and tissue levels in the dog evaluated. The PBPK model was capable of accurately predicting exhaled breath and blood levels in rats during and following inhalation exposure to TRI, TCE, and PCE. Of particular interest was the ability of the model to enable various degrees of accurate predictions in the seven different tissues monitored over time following halocarbon exposures. Predictions in rats and mice were fairly accurate, especially in highly perfused tissues. The first published PBPK model predictions in dogs provided in this study were less accurate, depending on the route of administration and dose employed. Therefore, the ability of the PBPK model to predict halocarbon concentrations in species of wide variation in size, for chemicals of varying degree of physicochemical properties, and over a spectrum of doses and routes of administration was demonstrated. Important interspecies differences in the kinetics and neurobehavioral toxicity of halocarbons have been determined and will be critical in determining the ultimate utility of interspecies extrapolations of toxicokinetic data for halocarbon using PBPK models.

THOMAS Mr. Russell Thomas Dr. Raymond Yang

AN INTERDISCIPLINARY AND ALTERNATIVE APPROACH TO ASSESS CARCINOGENICITY OF CHLOROBENZENES

The long term goal of this project is to develop an interdisciplinary approach in "Predictive and Alternative Toxicology" based on the integration of mechanistic toxicology and computer-based modeling systems [i.e., physiologically based pharmacokinetic/pharmacodynamic (PBPK/PD) models] for the evaluation of the carcinogenic activity of chlorobenzenes. The proposed studies will provide a greater knowledge of the roles of cell division and cell death in relation to chemically-induced cancer through the development of biologically-based cancer models. These models will reduce uncertainty in estimating the carcinogenic risk to humans from long-term exposure to chemical carcinogens and gain headway in the arena of low-dose extrapolation.

The proposed research will focus on 4 of the 12 isomers: 1,4-dichlorobenzene, 1,2,4,5-tetrachlorobenzene, pentachlorobenzene, and hexachlorobenzene. Chlorobenzenes are uniquely suited for this project because: (1) There is extensive basic biochemical, chemical, and toxicological information available on the selected isomers; (2) Adequate carcinogenicity bioassays have only been conducted 1,4-dichlorobenzene and hexachlorobenzene with limited carcinogenicity information available on 1,2,4,5-tetrachlorobenzene, providing a unique opportunity for predicting carcinogenicity of untested isomers, in this study, pentachlorobenzene; (3) Chlorobenzenes are very important industrial chemicals and environmental pollutants and are among the priority chemicals in the Air Force Installation Restoration Program and Bioenvironmental Hazards Program.

Our approach includes: (1) Conducting a thorough pharmacokinetic evaluation of selected isomers to assess target tissue dosimetry; (2) Evaluation of the carcinogenic activity of the four chlorobenzenes in the Ito's Medium-Term Bioassay using partially hepatectomized F344 rats and diethylnitrosamine as an initiator; (3) Parallel to Ito's Bioassay, perform "model-directed" experiments to define pharmacodynamic model parameters such as cell proliferation rates within normal liver cells and preneoplastic foci, cell death rates within normal liver cells and preneoplastic foci, and changes in cell-cycle kinetics using flow-cytometry measurements; (4) Correlating localized expression of transforming growth factor α , transforming growth factor β , and other biomarkers of cell proliferation in proliferating hepatocytes and preneoplastic nodules; (5) Integration of the above information into a PBPK/PD model to quantitatively assess the roles of cell division and cell death in relation to cancer and chlorobenzene exposure and formulate a predictive approach to assess carcinogenesis.

KRISHNAN Dr. Kannan Krishnan

A MOLECULAR STRUCTURE BASED MODELING FRAMEWORK FOR PREDICTING PHARMACOKINETICS OF ORGANIC CHEMICALS

The pharmacokinetic behavior of chemicals in biota is determined by certain chemical-specific and species-specific parameters. The chemical-specific parameters primarily refer to tissue:air, blood:air and tissue:blood partition coefficients (PCs). The species-specific parameters include cardiac output, alveolar ventilation rate, tissue volumes and tissue blood flow rates. Biochemical parameters such as absorption rates, binding constants, and metabolic rate constants are both chemical- and species-dependent. Physiologically-based pharmacokinetic (PBPK) models provide a framework to integrate the interrelationships among physiological, physicochemical and biochemical parameters to provide simulations of tissue dose of chemicals. PBPK models have been developed and validated for a limited number of volatile organic chemicals. There is an urgent need to develop mechanistic, predictive methodologies for a parameterization of PBPK models, to enable the use of these models early on in the product development and risk assessment processes. The objective of the present work is to develop a molecular structure based PBPK model framework for predicting the pharmacokinetics of organic chemicals. To forecast the pharmacokinetics and tissue dosimetry of untested organic chemicals, numerical values of the PCs and biochemical constants specific to a chemical in the species of interest are required. For predicting the PCs of organic chemicals, we have developed an algorithm based on tissue and blood composition data. Accordingly, the tissue:blood PCs are estimated by accounting for the relative solubility of chemicals in the neutral lipid, phospholipid, and water fractions in tissues and blood. This approach facilitates the characterization of each tissue compartment in the PBPK model as a mixture of neutral lipids, phospholipids, and water (instead of considering the model compartments as "empty" boxes as done conventionally). approach also enables the automated calculation of tissue:blood PCs from n-octanol and water solubility data, since these are approximated to solubility of chemicals in tissue/blood lipids and water. Using the present approach, the tissue:blood PCs could also be calculated within PBPK models by providing chemical structural information as input. Accordingly, each chemical is introduced into the model as a set of fragments (e.g., a methyl, carboxyl), each of which contributes a particular numerical value (i.e., a fragment constant) to the log n-octanol:water PC of the chemical. This datum is then used in the algorithm based on tissue and blood composition to predict tissue:blood PCs of chemicals within PBPK models. Future work in our laboratory will be directed toward the development and validation of methodologies for predicting the oral/dermal absorption constants, tissue diffusion coefficients, hemoglobin binding constants, and affinity and velocity of metabolism of organic chemicals from molecular structures. development and validation of a modeling framework to forecast tissue dosimetry and toxicity of chemicals based on their molecular structures should enhance our ability to choose and prioritize, from the multitude of chemicals available, the relatively "safer" ones for further detailed testing and potential use.

BASAK Dr. Subhash C. Basak

USE OF MOLECULAR SIMILARITY METHODS IN THE RISK ASSESSMENT OF CHEMICALS: A STUDY WITH QUADRICYCLANE

Risk assessment of chemicals is often carried out with limited or no experimental data. Frequently, no biological test data and empirical physicochemical properties necessary for hazard estimation are available. In the face of the paucity of data, the hazards posed by environmental pollutants is estimated using two major approaches; a) class specific quantitative structure-activity relationship (QSAR) models and b) structural analogs of toxicants.

In the first approach, a pollutant is assigned to a particular structural class and QSAR model for that class is used in estimating the hazard posed by the pollutant. But often a complex chemical cannot be placed into a particular class unequivocally. In such cases, the other viable alternative is to select analog(s) of the pollutant and use hazards of the analogs (or similar chemicals) to estimate the hazardous potential of the candidate chemical. Often the analogs are selected intuitively based on the individual judgment of the expert.

We have developed a number of methods for quantifying intermolecular similarity using nonempirical parameters. Such parameters can be calculated directly from molecular structure and can be computed for any arbitrary chemical species. Analogs are similar chemicals selected by such nonempirical techniques can be used for the hazard estimation of chemicals.

In this presentation we will discuss the development of a few molecular similarity methods. Use of quantitative molecular similarity analysis (QMSA) methods in estimating properties like boiling points, mutagenicity, octanol/water partition coefficient (logP) of various sets of molecules will be presented. We will also illustrate applications of QMSA methods in selecting analogs of quadricyclane from different and large data bases containing properties relevant to hazard assessment. Finally, we will compare relative efficacies of similarity methods vis-a-vis statistical and neural net methods in predicting properties.

MECHANISMS ASSOCIATED WITH THE TOXICITY OF POLYHALOGENATED CYCLIC HYDROCARBONS AND HEAVY METALS

Occupational exposure to structurally dissimilar polyhalogenated cyclic hydrocarbons (PCH) and heavy metals produce similar toxic effects including hepatotoxicity, neurotoxicity, progressive weight loss, and death. The cascade of events which occurs following exposure to these xenobiotics is not known, and therefore the mechanisms(s) of action of these toxicants has not been elucidated. Studies in our laboratories have demonstrated that PCH as lindane, TCDD, and endrin, and heavy metals as chromium and cadmium induce the production of reactive oxygen species in hepatic mitchondria and microsomes as well as peritoneal macrophages. Antioxidants/free radical scavengers can attenuate these effects. The urinary excretion of the lipid metabolites malondialdehyde, formaldehyde, acetaldehyde and acetone may be effective biomarkers of exposure to these xenobiotics. Preliminary studies have suggested that the activation of the protein kinase C second messenger system, release of the cytokine tumor necrosis factor-\alpha (TNF\alpha) and induction of stress/heat shock proteins occur in response to these diverse substances. We have hypothesized that the toxic manifestations are at least in part induced through a series of events involving the production of reactive oxygen species, activation of the protein kinase C system and release of TNFa. The sequence of these events is not known, and the relationship between these events and the induction of stress protein has not been studied. Both in vivo and in vitro effects on these parameters will be determined. Initial studies will be conducted in rats and mice using a single, oral, acutely toxic dose equivalent to one-half the LD₅₀ to provide a baseline for subsequent studies. In vitro studies will be conducted in macrophage J774A.1 and Chinese hamster ovary cell culture systems. Since most occupational exposure involves chronic, low doses, low dose chronic studies will be conducted. Dosing for up to 120 days will be conducted using a dose in the range of 1/10th-1/100th the acute dose. Animals will be sacrificed at 15 day intervals. Initial studies will focus on the identification and quantitation of biomarkers of toxicity including the urinary excretion of the lipid peroxidation products malondialdehyde; formaldehyde, acetaldehyde and acetone by HPLC, the production of reactive oxygen species by spectroscopic methods, an increased incidence of DNA single strand breaks by alkaline elution, enhanced production of TNFa, activation of the protein kinase C system, and induction of stress proteins by PAGE. Selected antioxidants/free radical scavengers and membrane stabilizers will be used to evaluate the role of reactive oxygen species in the activation of protein kinase C system, production of TNFa and induction of stress proteins. In summary, the results will greatly contribute to our knowledge of the mechanisms of toxicity of polyhalogenated cyclic hydrocarbons and heavy metals, and whether similar mechanistic pathways are involved. Information regarding biomarkers of exposure will be obtained, and the information will be exceedingly useful in developing strategies, and protocols for preventing and treating toxicities associated with occupational exposure to these xenobiotics.

CHROMIUM TOXICITY: REDUCTIVE ENZYMES IN HUMANS

Chromium (Cr) compounds are in wide use as components of many industrial processes and products. Exposure to Cr compounds can occur through occupational exposure, the environment, or the domestic use of Cr-containing products. Exposure to Cr compounds is associated with a wide array of toxic effects, including ulcerations, potentially serious damage to internal organs and increased incidence of certain cancers. The reductive metabolism of Cr(VI) to Cr(III), via reactive intermediates, is thought to play a key role in the cytotoxicity, mutagenicity, and potential carcinogenicity of Cr compounds. Studies on Cr(VI) reduction in human systems are scarce, and yet this information is central to understanding Cr toxicity and the potential for Cr-induced carcinogenesis in humans.

In rodents, microsomal enzymes are one class of cellular components which can mediate Cr(VI) reduction. Preliminary studies in our lab suggest that these rodent studies do not accurately reflect microsomal Cr(VI) reduction in humans. Based on our findings, we hypothesize that human microsomal enzymes can mediate Cr(VI) reduction at significant rates, at concentrations that are physiologically relevant, and under O_2 tensions typical for most well-oxygenated tissues. We further hypothesize that these Cr(VI)-reducing enzymes may irreversibly bind Cr as a result of Cr(VI) reduction and that this binding may disrupt their normal enzymatic role. Finally, we hypothesize that microsomal flavoenzymes (e.g. P450 reductase and flavin-containing monooxygenase), are likely candidates as the major microsomal Cr(VI)-reducing enzymes.

The specific aims of this proposal are to examine Cr(VI) reduction by human microsomes in order to: (1) determine the general characteristics of Cr(VI) reduction by human microsomal enzymes, including determination of both the kinetic aspects of, and interindividual differences in, microsomal Cr(VI) reduction; (2) elucidate the effects of various levels of O_2 on human microsomal Cr(VI) reduction; (3) examine the potential irreversible binding of Cr to microsomes as a result of Cr(VI) reduction, and the potential effects of this binding on microsomal enzyme activities; and (4) determine the ability of key microsomal enzymes, including NADPH:cytochrome P450 reductase and flavin-containing nonooxygenase(s), to mediate Cr(VI) reduction.

Together, these studies will provide necessary and important insight into the potential mechanisms of human microsomal Cr(VI) reduction and hence into the cytotoxicity, genotoxicity, and carcinogenicity of Cr(VI) compounds in man.

OXIDATIVE STRESS, GAP JUNCTIONAL COMMUNICATION AND EPIGENETIC TOXICOLOGY

Gap junctional intercellular communication (GJIC) is a fundamental biological process in all multicellular organisms which has been implicated in the regulation of cell proliferation. differentiation and adaptive responses of differentiated cells. Disruption of GJIC by many nongenotoxic chemicals and oncogenes has been linked to several disease endpoints, including teratogenesis, tumor promotion, reproductive and neurotoxicological dysfunctions. The goal of this proposal is to continue our studies on the mechanisms by which toxic chemicals can block GJIC, particularly those that induce oxidative stress in both human and rodent cells, in vitro and selected chemicals of interest to the AFOSR (namely tetracycloheptone, fluorocarbon ethers, and ammonium dinitramide). The specific aims will be to determine (a) if a series of known toxic chemicals can inhibit gap junctional intercellular communication (GJIC) in several human and rat cell lines: and (b) if the generation of free radical oxygen species is responsible, via some mechanism, for altering GJ function. GJIC will be measured using the scrape loading/dyetransfer fluorescent recovery after photobleaching (FRAP) and microinjection - FRAP techniques. The mechanisms by which chemicals block GJIC will be tested at the transcriptional translational and posttranslational levels using molecular biological/biochemical techniques (northerns, westerns, in situ immunofluorescence) with probes for the gap junction genes and antibodies for the connexin proteins.

The test of the hypothesis that these toxic chemicals which block GJIC also block programmed cell death or apoptosis will also be made. Finally, a series of biochemical/fluorescent imaging techniques to determine the specific mechanism by which oxidative-stress inducing toxic chemicals block GJIC will be utilized. The significance of these studies will be to understand the detailed manner by which important toxic chemicals block GJIC to lead to various diseases in order that specific remediation/chemoprevention strategies can be devised. The specific experimental approach will involve various toxic chemicals (e.g., dichloroacetic acid; trichloroacetic acid; chloral; quadricyclane; chromium salts; cyanide; naphthalene; ethylene glycol; 2,6-dinitrotoluene, etc.) which will be placed on human kidney epithelial, rat liver epithelial and glial cells, at non-cytotoxic levels to determine if gap junctional intercellular communication (GJIC) will be inhibited. If any of these chemicals are found to block GJIC, various assays to determine (a) if radical oxygen species are generated (fluorescence detection with 2.7-dichlorofluorescein in the presence of selected free radical scavengers; spin trapping); (b) to determine if a change in the oxidative status of a cell results from changes in the intracellular levels of anti-oxidant mechanisms (i.e., GSH, GSH peroxidase, ascorbate, a tocopherol, catalase); (c) the potential biochemical mechanisms(s) by which free radicals inhibit

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GJIC (e.g., alterations in intracellular free Ca++ or pH; activation of phosphorylation/de-phosphorylation of gap junction proteins, etc.). This in vitro model to study both basic mechanisms and development of protective measures can also reduce the need for animal toxicity studies. As part of these studies, comparative effects of those toxic chemicals of concern to the USAFOSR on GJIC in both human and rodent cells in vitro, as well as cells from different organs (e.g., skin, liver, brain, etc).

DEPLETION OF NUCLEAR POLY (ADP-RIBOSE) POLYMERASE BY ANTISENSE RNA EXPRESSION: INFLUENCES ON DNA REPAIR AND REPLICATION, GENOMIC STABILITY, AND SURVIVAL OF CELLS TO GENOTOXIC AGENTS

Poly(ADP-ribose) polymerase (PADPRP) is a chromatin-bound enzyme which is pivotal in cellular recovery from DNA strand break damage. Three additional years of research support is requested from the AFOSR for our program which concerns, first, the use of biotechnology and molecular biology approaches towards the elucidation of the biochemical mechanisms by which this enzyme mediates repair of cells from specific environmental toxic agents, of interest to AFOSR and secondly, in a practical vein, to experimentally exploit the properties of this enzyme and its product, poly(ADP-ribose) to develop new Biomarker assays to be used in collaboration with intramural AF laboratories as a novel assessment of environmental hazards.

PADPRP requires DNA for activity, and it is significant that the catalytic activity of this enzyme is directly coordinated with the <u>number</u> of DNA strand breaks in DNA, both <u>in vitro</u> as well as <u>in vivo</u>. Thus, poly(ADP-ribosyl)ation is rapidly modulated in response to environmentally significant, DNA-damaging agents; it probably represents the most initial response of the cell to genotoxic damage to the genome. Accordingly, significant reductions in cellular NAD levels reflect increased poly(ADP-ribosyl)ation due to DNA strand breaks. Hence, it is of significance to this application that Proctor and Casida showed that 38 organophosphorus and methyl carbonate <u>insecticides</u> in doses as low as 0.6 parts per million cause lowering of NAD. The levels of NAD were directly correlated with <u>teratogenesis</u> in this study.

Our laboratory, during earlier AFOSR granting periods, was the first to isolate and clone a fulllength cDNA for PADPRP. In subsequent years, our experiments focused on understanding how poly(ADP-ribosyl)ation affects chromatin structure overall and DNA repair and replication specifically. For these studies, we developed several biochemical and immunological techniques and assays, many of which continue to be useful in the proposed future continuation. More recently, we have also provided a variety of molecular biology techniques. One of the major aims over the past few years of this project has been to establish and characterize cells stably transfected with PADPRP antisence cDNA under the control of an inducible promoter and to establish conditions under which significant depletion of nuclear PADPRP could be achieved. This approach has been particularly successful in assessing the potential roles of poly(ADPribosyl)ation in a variety of biological processes, all involving DNA strand breaks, without the use of non-specific chemical inhibitors. Thus, we have assigned biochemical roles for PADPRP in the recovery of cells with exposure to mutagenic agents, gene amplification and DNA replication. These past studies should allow us to learn considerably more about the mechanism role of this enzyme in cells exposed to stressful environments, and also to the development of more practical Biomarker assays, coupled with this reaction.

Accordingly, in AIM I of the renewal program, we propose to exploit the experimental protocols established during the last granting period with HeLa cells transfected with PADPRP antisense RNA constructs to further study the role of this enzyme in DNA repair, strand rejoining reactions, and chromatin reassembly in other cell systems, appropriate to environmental agents of interest to AFOSR (i.e. ADN, hydrazine, trichloroethylene, tetrochloroethylene, N-Nitrosodimethylamine, and cadmium, etc.). For example, a novel human immortalized karytinocyte cell line transfected with antisense to PADPRP has been developed in pilot studies, since skin is one tissue at high risk to exposure to a number of environmental agents. These engineered skin tissue culture cells have been grafted onto mice and form a layer of human skin, which is histologically identical to normal skin, then, using new Biomarker methods, piloted in AIM II, we have shown that topical addition of an alkylating agent (as a prototype for other agents) elicits rapid synthesis of poly(ADP-ribose) polymer (an indirect measure of DNA breaks). Other types of cells and organs will be tested in AIM I. we will also determine whether sufficient PADPRP-DNA-binding domain can also be induced (in various cells) as an alternative method to inhibit endogenous nuclear polymerase activity completely.

The experiments projected in AIM II are a logical extension of the biology and biochemistry information gained in AIM I. These new approaches represent a practical utilization of this information by developing two new Biomarker assays for the assessment of environmental hazardous agents. Observations relevant to this aim include the following: (a) The biosynthesis of the unique biopolymer, poly(ADP-ribose) is one of the earliest responses of cells to DNA damage, as elicited by many environmental hazardous agents; (b) The DNA-binding Domain of PADPRP is among the most effective cellular proteins which binds to both single and double strand DNA breaks. Our laboratory, during the last period, has overexpressed this human protein in bacteria. We propose to develop two new Biomarker assays, of which preliminary data suggests a high level of feasibility. On the one hand, we will develop a bioassay using the ability of antibody, specific to poly(ADP-ribose) polymer to detect this product (and indirectly DNA damage) on fixed cells or tissues. Secondly, we will develop a similar type of assay to detect DNA strand breaks in tissues cells or tissues by the unique binding of the PADPRP-DBD on fixed slides or tissues which have been exposed to hazardous agents and subsequently the detection of this bound protein only to DNA ends by immunological procedures.

WITZMANN Dr. Frank A. Witzmann

TWO-DIMENSIONAL PROTEIN PATTERN RECOGNITION IN CHEMICAL TOXICITY

The Air Force Program in Toxicology is interested in developing a more proactive approach to toxicity testing, one based on predictive toxicology. Through our interaction with the Toxicology Division of the Armstrong Laboratory and the unique capabilities we possess, our laboratory is developing a predictive toxicology based on pattern recognition. By using two-dimensional electrophoresis of proteins (2D-PAGE), we are developing methods for comparing computerrecognized 2D-protein pattern alterations in various target tissues induced by specific chemical agents to quickly, economically, and reliably assess and predict hepatoxicity, nephrotoxicity, or immunotoxicity, etc., as well as toxic mechanism. The strength of the large-scale 2D-PAGE technique lies in its ability to resolve literally thousands of cellular proteins in a single sample, first based on their content of acidic and basic amino acids (isoelectric focusing), and second by molecular weight (SDS electrophoresis). In combination, these two separation techniques produce a two-dimensional protein pattern unique for each tissue or group of cells tested. Individual proteins within the pattern can be analyzed for alterations in volume (density), charge, and molecular weight. Changes in volume or spot density reflect alterations in a protein's abundance and suggest up- or down-regulation of the genome or altered protein turnover rates. Charge modifications suggest either posttranslational modification or point mutations in the genome. Regardless of the type of changes observed, a well-resolved 2D protein pattern, or 2D protein map (fingerprint), provides a pattern realistically containing 1000-2000 proteins and is thus a significant source of information regarding the health/activity of a particular cell/tissue type. With the advent of user-friendly computerized imaging of the protein patterns generated by 2D-PAGE and its use in pattern recognition for animal model target tissues, 2D-PAGE has become an even more powerful technique in toxicity testing; one with increasingly welldocumented potential.

A MECHANISTICALLY BASED, IN VITRO EVALUATION OF OCULAR IRRITANTS

There are currently more than 40 published in vitro tests for predicting the ocular irritancy potential of test substances. Although these tests range in complexity, they all share the major obstacle of validation in predicting the in vivo ocular response. Our research team has developed three dimensional, in vitro organotypic models for the rabbit and human anterior cornea which we believe will provide information necessary to address the problem of assay validation. The organotypic models (corneal equivalents) consist of a collagen-based stromal matrix which is supported by a polycarbonate membrane and contains rabbit corneal keratocytes and epithelial cells. The corneal epithelial cells are grown on top of the stromal matrix and allowed to differentiate into basal, wing and superficial epithelial layers. The resulting three dimensional models are histologically and biochemically analogous to their respective native tissues.

Tissue isoelectric focusing (TIF) techniques developed in our laboratory will be used to establish comparative biochemical profiles for structural and functional proteins isolated from rabbit and human comeas and their respective corneal equivalents. Histomorphometric data will be obtained from corneal equivalents and native rabbit and human corneas for immunoreactivity against several biomarkers of ocular irritation including: interleukin-1-alpha, fibronectin, intercellular adhesion molecule-1, heat shock protein 70 and lactate dehydrogenase. The combination of characteristic protein profiles for structural and functional proteins and the histomorphometric data for biomarkers of tissue injury will be used to establish a reference database for the corneal equivalents and the native tissues.

Corneal equivalents will be exposed to chemicals in vitro and protein biomarkers of the irritant-tissue interaction identified to alterations in the TIF and histomorphometric data when compared to the reference database. TIF and histomorphometric data will be used to: (1) rank the severity and establish a dose-response relationship for the ocular irritants, (2) explore the mechanism of selected ocular irritants and (3) directly compare the irritant response of rabbit and human organotypic models. The major goal of the proposed study is to develop the rabbit and human organotypic models as animal use alternatives in the toxicologic evaluation of compounds used by the U. S. Air Force. In addition, the use of human corneal equivalents in the in vitro exposure protocols will provide a unique basis for the extrapolation of ocular irritancy data to the potential human response.

NMR SPECTROSCOPY AS A TOOL FOR STUDIES OF HEPATOTOXICITY IN VIVO

Nuclear magnetic resonance (NMR) spectroscopy is a useful tool for studies of tissue metabolism in vivo, and as such, opens a new realm of exploratory possibilities in toxicology research. This methodology provides a window into the pathways of tissue biochemistry, and enables one to assess the effects of xenobiotics on endogenous metabolism and tissue function. Such studies may reveal early predictors of toxicity which is not possible through conventional toxicology testing, and can aid in our understanding of toxicological mechanisms.

This presentation will describe our research concerning the hepatotoxicity associated with perfluorocarboxylic acids, specifically perfluoro-n-octanoic acid (PFOA) and perfluoro-n-decanoic acid (PFDA). These fluorocarbons belong in a class of compounds collectively known as peroxisome proliferators (PPs). This structurally diverse group of compounds covers a range of commercial and biological utility. Unfortunately, many PPs display severe toxicity and are nongenotoxic hepatocarcinogens; the mechanisms of action are not understood.

NMR studies from our laboratory have revealed that perfluorocarboxylic acids are not metabolized, yet cause significant effects on hepatic carbohydrate and phospholipid metabolism. Following PFDA treatment in rats hepatic effects included: decreased glucose utilization, inhibition in glycogenesis, decreased utilization of glucogenic amino acids (i.e., alanine), and a significant increase in liver phosphocholine. Standard biochemical analyses have confirmed that the effect on PCho concentration is the result of an activation in liver phospholipase C. Diacylglycerol, an important second-messenger metabolite, is also significantly elevated. These results suggest that PFDA, and other PPs, may induce various metabolic effects through a mechanism involving protein kinase C activation.

Our experimental results demonstrate the utility of NMR techniques in toxicology research, and aid in our understanding of the impact of PPs on liver function. Future studies will characterize the effects of various other PPs on liver phospholipid metabolism, in an effort to delineate a common biochemical mechanism of action.

RISBY Dr. Terence Risby

BIOMARKER ANALYSIS OF HUMAN BREATH FOR EARLY PREDICTION OF HEPATOTOXICITY

More than 500,000 people are occupationally exposed to tetrachloroethylene, a cleaning and degreasing solvent that is a suspected hepatotoxin. Early signs of hepatotoxicity from this agent have been difficult and expensive to detect. We propose that assessment of the risk to human health posed by realistic occupational levels of tetrachloroethylene can be made rapidly and non-invasively based on quantitative molecular epidemiology using breath biomarkers of exposure and effect.

The specific aims of this study are to: 1) identify and quantify breath sulfur-and nitrogen-containing biomarkers of liver dysfunction; 2) generate a library of these breath biomarkers for various liver diseases; 3) investigate whether increased free radical generation, as measured by levels of breath ethane, occurs as a result of a 4 hour exposure to occupational levels of tetrachloroethylene; 4) investigate whether CNS toxicity, as measured by airway occlusion pressure, occurs as a result of a 4 hour exposure to occupational levels of tetrachloroethylene; and 5) demonstrate that breath biomarkers can be used to identify people who have liver dysfunction as a result of occupational exposure to tetrachloroethylene.

ROBLEDO Mr. Raymond Robledo Dr. Mark Witten

THE CHRONIC EFFECTS OF JP-8 JET FUEL EXPOSURE

In a simulated military flightline exposure protocol, male congenic mice and their male C57BL6 parent strain were used to investigate the pulmonary effects of aerosolized JP-8 jet fuel The congenic mice are deficient in the induction of both aryl hydrocarbon hydroxylase (AHH) and N-acetyltransferase (NAT) enzymes. Congenic mice (MHD) were exposed nose-only daily for one hour to a 1,036 mg/m³ average of JP-8 for seven days with comparison to C57BL6 mice (BHD) similarly exposed to 1,092 mg/m³ average of JP-8 and their corresponding baseline control groups (MBC=congenic, BBC=C57BL6). JP-8 jet fuel exposure caused a significant increase in alveolar epithelial clearance to the MHD (1.22 %/min) group compared to MBC (0.44 %/min), BBC (0.38) %/min) and BHD (0.23 %/min) groups, as measured by technetium labeled diethylenetriamine pentaacetate (99mTcDTPA) clearance. Increased alveolar epithelial clearance to the MHD group was supported by a significant increase in bronchoalveolar lavage fluid (BALF) total protein (74.34 µg/ml) over MBC (35.83 µg/ml), BBC (34.78 µg/ml) and BHD (34.57 µg/ml) groups. Light microscopy showed pathological signs of alveolar edema, red blood cell infiltration, and airway inflammation for MHD as compared to all groups. The MHD group also showed a significant increase in pulmonary compliance, which was not accompanied by significant total pulmonary resistance changes with respect to its control. The pulmonary changes do not appear to be a systemic immune response, as total leukocyte counts in BALF remained unchanged. In order to determine a possible role for the neuropeptide substance P in lung injury, congenic mice were exposed similarly to 1,000 mg/m³ followed by 15 minutes of aerosolized 1 µM substance P (MHP) for seven days with a corresponding control group (SPC). MHP (0.461 %/min) had significantly lowered 99m Tc-DTPA clearance along with a significant decrease in BALF total protein (35.24 µg/ml), compared to Substance P also reduced pathological lung injury as determined by light microscopy. The attenuation of lung injury by substance P may be mediated through an immune response as MHP (2.04 x 10⁴) had significantly lower total cells in BALF as compared to MHD (3.88 x 10⁴). Supported by USAFOSR F49620-94-1-0297 and DOD AASERT Program.

IMMUNOTOXICOLOGY OF EXPOSURE TO JP-8 JET FUEL AND HALOGENATED HYDROCARBONS

Inbred C57BL6 mice were exposed to either 500, 1000 or 2500 mg of aerosolized JP-8 for a period of 7 days, 1 hour of exposure per day. 24 hours after the last exposure the animals were sacrificed and the effects of exposure on the immune system examined. Immune organs (spleen, thymus, blood, lymph nodes and bone marrow) were recovered and analyzed for effects on organ weight, total cell numbers, immune cell populations (by differentials), and lymphocyte subpopulations (by flow cytometry). Assays were also performed to examine the effects of exposure on immune function. Exposure to JP-8 was found to significantly decrease the total cell numbers in spleen and thymus of the animals, even at the lowest doses utilized. Flow cytometric analyses revealed that all lymphocyte subpopulations were affected equally, although it appeared that exposure resulted in an increase in inflammatory cells. Similar effects on immune cell subpopulations were also observed in lymph nodes. In the thymus it appeared that the immature CD4+CD8+ cells were differentially lost due to exposure. In terms of immune function, JP-8 exposure resulted in a significant and profound suppression in immunological competence as assessed by mixed lymphocyte reactions to mitogens, which could not be overcome by the addition of exogenous growth factors (i.e., IL-2), at even the lowest dose of exposure. An opposite effect was observed for responses to growth factor (IL-2) alone, indicating that exposure may have initiated an inflammatory reaction. Interestingly, treatment of the exposed animals with Substance P invariably reversed the effects on all measured parameters of JP-8 exposure to almost normal levels. Thus, it appears that exposure of animals to even low doses of JP-8 has a significant suppressive effect on the immune system in terms of both immune cell numbers and immune cell function. However, it may be possible to prevent or reverse these effects by treatment of the animals with Substance P

SIEGEL
Dr. Frank L. Siegel
Dr. Steven Kornguth

DETOXICATION ENZYMES AS BIOMARKERS OF TOXIN EXPOSURE

Our laboratories have been investigating toxin-related changes in the expression of isoenzyme forms of the detoxication enzyme glutathione S-transferase (GST) in rodents and in human blood cells and plasma. GSTs are putative biomarkers of toxicant exposure. GST is a superfamily of about fifteen isoenzymes, each a separate gene product. GSTs are classified into four families (alpha, mu, pi and theta). The members of each family form homo- and heterodimers and share substrate specificity as well as a high degree of amino acid sequence homology. GSTs in liver are induced by carcinogens, antioxidants, dioxin, phenobarbital and other antioxidants. We have described an hplc method for quantitating the level of each GST isoenzyme in small tissue samples and methods for the sensitive cellular localization of specific GSTs by immunohistochemistry. We have mapped GST isoenzymes in brain and kidney and have found that a given cell type has a characteristic profile of GST isoenzymes. The effects of bilirubin (a neurotoxin), inorganic lead, triethyllead, JP-8 jet fuel and trichloroethane on the expression of GST isoenzymes were determined and the results indicate that GSTs are tissue biomarkers of toxin exposure. In brain, GSTs were formerly believed to be localized in non-neuronal cells; our results provide evidence for high levels of GST in cerebellar Purkinje cell neurons. In the Gunn rats, a mutant which has high levels of bilirubin due to a genetic defect, massive cell loss is seen in the central portion of cerebellum (vermis) while lateral lobes of the cerebellum are spared. In these non-vulnerable brain regions, bilirubin caused large increases in specific GSTs; these GST effects were not seen in the vermis, suggesting that GST induction is a protective adaptation. Acute and chronic exposure to inorganic lead, a toxin with primary effects on kidney, caused increases in specific GST isoenzymes; these GST increases preceded irreversible pathobiological changes in renal structure and function. Lead-related increases in kidney GST expression were dramatically exacerbated by modest reduction of dietary calcium. Dose response the time course studies of the effects of a single i.p. injection of triethyllead on GSTs in kidney, liver and whole brain and retina have been completed. Biochemical, immunohistochemical, electron microscopic and light microscopic analyses of kidney from triethyllead-treated rats are nearing completion. A single acute exposure to triethyllead caused dramatic changes in behavior, animals became very aggressive toward one another. Most kidney GST isoenzymes increased after a single i.p. injection of triethyllead (10 mg/kg). Triethyllead caused increases in specific GST isoenzymes at much lower doses than were required of inorganic lead. The pathobiological effects of organic lead in kidney differ from those previously seen with inorganic lead. The decline in specific liver GSTs is a novel effect; immunohistochemical studies now underway are designed to tell us if this decline represents the loss of specific cell type in liver which is enriched in the specific GST isoforms whose levels declined following triethyllead administration, GST isoenzymes were also mapped in retina and characteristic changes were shown to result from triethyllead exposure. A pilot study of GST isoforms in blood fractions from Hill Air Force personnel has been completed. This study demonstrated the feasibility of GST analyses on blood

samples transported from Hill AFB to our laboratory and analyzed 24 h after the blood samples were drawn. The GST activities in red blood cells, white blood cells and plasma were shown to be independent measures, probably reflecting unique isoenzyme distribution in these fractions. When blood plasma alpha class GST levels in 16 control Air Force personnel were compared to values from 16 Air Force personnel who were working with jet fuel, one of the exposed group had GST levels five times greater than the upper limits of the normal range, suggesting that this measure may be an effective exposure biomarker.

AFOSR

PREDICTIVE TOXICOLOGY PROGRAM REVIEW

31 May - 1 June 1995

Holiday Inn Conference Center/I-675 Fairborn, Ohio

SPEAKERS

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Mr. Mehdi Adinehzadeh WSUSOM/Cox Institute Kettering, OH

Dr. William O. Berry AFOSR/NL Bolling AFB, DC

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AIR FORCE NONLINEAR OPTICAL POLYMERS CONTRACTORS REVIEW MEETING

Holiday Inn I-675 Conference Center, Fairborn, OH 26 February-28 February 1996

SUNDAY, 25 FEB 1996

3:00-7:00pm:

Registration

MONDAY, 26 FEB 1996

7:00-8:00am:

Registration/Continental Breakfast

INTRODUCTION

8:00-8:30am:

FUTURE DIRECTIONS OF AFOSR NLO POLYMER PROGRAM

Charles Lee, AFOSR, Chair

8:30-9:00am:

GUIDED-WAVE E-O DEVICES: WHERE IS THE ACTIVE MATERIAL?

F. Kenneth Hopkins, WL/MLPO

9:00-9:30am:

COCKPIT APPLICATIONS

Darrel Hopper, WL/AAA

9:30-9:50am:

FREQUENCY CONVERSION PHENOMENA WITH POLED POLYMERS

George Stegeman, University of Central Florida

9:50-10:10am:

BREAK

F. Kenneth Hopkins, WL/MLPO, Chair

10:10-10:30am: FABRICATION AND LOSS MEASUREMENTS OF ETCHED

POLYMER EO WAVEGUIDE DEVICES William Steier, University of Southern California

10:30-11:00am: NONLINEAR DISPERSION AND FEMTOSECOND EXPERIMENTS IN

EPITXIALLY GROWN PHYTHALOCYANINES AND OTHER ORGANICS

Nasser Peyghambarian, University of Arizona

11:00-11:30am: ELECTRO-OPTIC POLYMER DEVELOPMENT

Susan Ermer, Lockheed Martin Research and Development

11:30-12:00am: ELECTRONIC OSCILLATOR APPROACH TO OPTICAL

NONLINEARITIES IN CONJUGATED POLYMERS

Shaul Mukamel, University of Rochester

12	:00-	1:0	0pm
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LUNCH

	Raymond Boncek, RL/OCPA, Chair		
1:00-1:30pm:	CURRENT AF EFFORTS IN PHOTONICALLY IMPLEMENTED RF PHASED ARRAYS: THEORY AND PRACTICE Norman P. Bernstein, RL/OCPC		
1:30-2:00pm:	ELECTRO-OPTIC POLYMER DEVELOPMENT II - SUMMARY Robert Gulotty, The Dow Chemical Company		
2:00-2:30pm:	BIPOLARONIC CHARGE STATE INCORPORATION IN NONLINEAR OPTICAL MATERIALS AND POLYMERS Charles W. Spangler, Northern Illinois University		
2:30-3:00pm:	A SYSTEMATIC APPROACH TO ENHANCE THE THIRD ORDER POLARIZABILITY OF SQUARAINE DYES Carl Dirk, University of Texas		
3:00-3:20pm:	BREAK		
Tom Cooper, WL/MLPJ, Chair			
3:20-3:50pm	OPTOELECTRONIC DEVICES James Grote, WL/AA		
3:50-4:20pm:	OPTICAL INTERCONNECTS RELATED TO BOARD LEVEL OR LOCAL LEVEL COMMUNICATIONS Ray Boncek, RL/OCP		
4:20-4:50pm:	HIGH PERFORMANCE POLYMERS FOR ELECTRO-OPTIC APPLICATIONS Alex Jen, ROI Technology.		
4:50-5:20pm:	CURRENT PROGRESS IN X ⁽³⁾ STUDIES Anthony F. Garito, University of Pennsylvania		
5:20-5:40pm:	CURRENT PROGRESS IN X ⁽²⁾ STUDIES Anthony F. Garito, University of Pennsylvania		
5:40-6:00pm:	THIRD ORDER NLO RESPONSE OF DIFFUSE CHEMICAL SYSTEMS Douglas S. Dudis, WL/MLBP		
6:30-8:30pm:	Evening Social at Holiday Inn		

TUESDAY, 27 FEBRUARY 1996

12:00-1:00pm:

TUESDAT, 27 FEBRUARY 1996		
7:15-8:00am:	CONTINENTAL BREAKFAST	
	Stephen Caracci, WL/MLPO, Chair	
8:00-8:30am:	RECENT ADVANCES IN THE DESIGN OF NLO MATERIALS Seth R. Marder, California Institute of Technology	
8:30-9:00am:	NEW APPROACHES TO GROWTH OF HIGHLY OPTICALLY NONLINEAR ORGANIC THIN FILMS Stephen R. Forrest, Princeton University	
9:00-9:30am:	PROGRESS TOWARD POLYMER OPTOELECTRONICS APPLICATIONS Alan J. Heeger, University of California	
9:30-9:50am:	PROGRESS TOWARDS DEVELOPING A LOW LOSS ELECTRO-OPTIC POLYMER IN THE NEAR IR William K. Bischel, Deacon Research	
9:50-10:10am:	BREAK	
	R. J. Spry, WL/MLBP, Chair	
10:10-10:30am:	ELECTRIC FIELD EFFECTS IN POLYMERS FOR SECOND ORDER NLO Hilary L. Lackritz, Purdue University	
10:30-11:00am:	DESIGN, SYNTHESIS, AND PERFORMANCE OF ADVANCED NLO-ACTIVE MOLECULAR ASSEMBLIES Tobin J. Marks, Northwestern University	
11:00-11:30am:	MECHANISMS OF THIRD ORDER OPTICAL NONLINEARITY IN QUASI-ONE AND TWO DIMENSIONAL ORGANIC SYSTEMS Sumit Mazumdar, University of Arizona	
	THE NEEDS OF ANALOG & DIGITAL NETWORKS IN FUTURE AVIONICS ARCHITECTURES Joseph S. Wilgus, WL/AAA-1	

LUNCH

Stephen Caracci, WL/AA, Chair

1:00-1:30pm:	NONMECHANICAL BEAM STEERING Philip Douville, WL/AAWW-3
1:30-2:00pm:	MATERIALS REQUIREMENTS FOR OPTICAL LIMITING APPLICATIONS Patrick Hood, WL/MLPO
2:00-2:30pm:	PROGRESS IN THERMALLY AND TEMPORALLY STABLE ELECTRO- OPTIC POLYMERS WITH WIDE OPTICAL TRANSPARENCY (SECOND ORDER NLO) Paras N. Prasad, State University of New York
2:30-3:00p.m:	RESONANT X ⁽³⁾ PROCESSES-TWO PHOTON LASING AND OPTICAL POWER LIMITING Paras N. Prasad, State University of New York
3:00-3:20pm:	BREAK
	Douglas S. Dudis, WL/MLBP, Chair
3:20-3:40pm:	AF MATERIALS RESEARCH IN SUPPORT OF OPTICAL LIMITING Richard L. Sutherland, SAIC
3:40-4:00pm:	2ND ORDER NLO POLYMER PROCESSING AND CHARACTERIZATION AT WPAFB Stephen Caracci, WL/MLPO
4:00-4:30pm:	ADVANCES IN PHTHALOCYANINES FOR OPTICAL LIMITING Joe Perry, California Institute of Technology
4:30-5:00pm:	ADVANCES IN SYNTHESIS AND PROCESSING OF SECOND-ORDER NONLINEAR OPTICAL MATERIALS Larry R. Dalton, University of Southern California
5:00-520pm:	THERMAL STABILITY OF SECOND ORDER NLO CHROMOPHORES Ivan J. Goldfarb, Wright State University
5:20-5:40pm:	ETALON-BASED CHARACTERIZATION AND PROBING OF HIGH-SPEED ELECTRONIC CIRCUITS WITH ELECTRO-OPTIC POLYMERS Vince Dominic, University of Dayton

WEDNESDAY, 28 FEBRUARY 1996

7:15-8:00am:

CONTINENTAL BREAKFAST

John Zetts, WL/MLPO, Chair

8:00-8:30am:

SPACE COMMUNICATIONS

Carl Gass, PL/VTRA

8:30-9:00am:

IMAGE PROCESSING

Charles Woods, RL/EROP

9:00-9:30am:

SYNTHESIS AND CHARACTERIZATION OF 2-PHOTON RESONANT

THIRD-ORDER NLO MATERIALS Bruce A. Reinhardt, WL/MLBP

9:30-:950am:

SYNTHESIS OF 2ND-ORDER NLO CHROMOPHORES AND POLYMERS

FOR EO APPLICATIONS Bruce A. Reinhardt, WL/MLBP

9:50-10:10am:

BREAK

Patrick Hood, WL/MLPO, Chair

10:00-10:30am: THERMAL STABILITY IN ELECTRO-OPTIC POLYMERS

Kenneth D. Singer, Case Western University

10:30-11:00am: FABRICATION AND TESTING HIGH SPEED ELECTRO-OPTIC

POLYMER MODULATORS FOR FIBER-OPTIC DATA LINK

APPLICATIONS

Yongqiang Shi, TACAN Corporation

11:00-11:30am: PICOSECOND ALL-OPTICAL SWITCHING USING OFF-RESONANT

NONLINEAR REFRACTIVE INDEX OF PTS

Mrinal Thakur, Auburn University

11:30-12:00am: SPACE APPLICATIONS

Karl W. Koch, PL/LIDN

12:00-1:00pm:

LUNCH

Darrell Hopper, WL/AA, Chair

1:00-1:30pm:	VERY LOW LOSS INTEGRATED WAVEGUIDES OF PMMA, DBR FILTER EFFECTS AND IR TWO-PHOTON PUMPED BLUE UPCONVERSION WAVEGUIDE LASERS Anadi Mukherjee, Laser-Matter Interaction Laboratories, Inc.	
1:30-2:00pm:	HIGH TEMPERATURE NLO POLYMERS Robert Miller, IBM Almaden Research Center	
2:00-2:30pm:	POLYMER ELECTRO-OPTIC DEVICES AND PROCESSES John Kenney, ROI Technology	
2:30-3:00pm:	MULTICOLOR LITHOGRAPHY FOR REFRACTIVE INDEX GRADIENT FABRICATION Robert Mustacich, RVM Scientific, Inc.	
3:00-3:20pm:	BREAK	
Bruce A. Reinhardt, WL/MLMP, Chair		
3:20-3:40pm:	LD3-NLO-POLYMER-BASED GUIDED WAVE DEVICES Ray Chen, University of Texas	
3:40-4:10pm:	POLYMER-BASED GUIDED-WAVE WAVELENGTH DIVISION MULTIPLEXER FOR NETWORK APPLICATIONS Ray Chen, University of Texas	
4:10-4:40pm:	IMPROVING THE SYNTHESIS OF NLO CHROMOPHORES AND POLYMERIC MATERIALS William Feld, Wright State University	
4:40-5:10pm:	PROGRESS IN ELECTROOPTIC POLYMERS AND COMPOSITES Ryszard Burzynski, Laser Protonics Technology	
5:10-5:20pm	CLOSING REMARKS	

Stephen Caracci, WL/AA, Chair

1:00-1:30pm:	NONMECHANICAL BEAM STEERING Philip Douville, WL/AAWW-3
1:30-2:00pm:	MATERIALS REQUIREMENTS FOR OPTICAL LIMITING APPLICATIONS Patrick Hood, WL/MLPO
2:00-2:30pm:	PROGRESS IN THERMALLY AND TEMPORALLY STABLE ELECTRO- OPTIC POLYMERS WITH WIDE OPTICAL TRANSPARENCY (SECOND ORDER NLO) Paras N. Prasad, State University of New York
2:30-3:00p.m:	RESONANT X ⁽³⁾ PROCESSES-TWO PHOTON LASING AND OPTICAL POWER LIMITING Paras N. Prasad, State University of New York
3:00-3:20pm:	BREAK
	Douglas S. Dudis, WL/MLBP, Chair
3:20-3:40pm:	AF MATERIALS RESEARCH IN SUPPORT OF OPTICAL LIMITING Richard L. Sutherland, SAIC
3:40-4:00pm:	2ND ORDER NLO POLYMER PROCESSING AND CHARACTERIZATION AT WPAFB Stephen Caracci, WL/MLPO
4:00-4:30pm:	ADVANCES IN PHTHALOCYANINES FOR OPTICAL LIMITING Joe Perry, California Institute of Technology
4:30-5:00pm:	ADVANCES IN SYNTHESIS AND PROCESSING OF SECOND-ORDER NONLINEAR OPTICAL MATERIALS Larry R. Dalton, University of Southern California
5:00-520pm:	THERMAL STABILITY OF SECOND ORDER NLO CHROMOPHORES Ivan J. Goldfarb, Wright State University
5:20-5:40pm:	ETALON-BASED CHARACTERIZATION AND PROBING OF HIGH-SPEED ELECTRONIC CIRCUITS WITH ELECTRO-OPTIC POLYMERS Vince Dominic, University of Dayton

WEDNESDAY, 28 FEBRUARY 1996

7:15-8:00am:

CONTINENTAL BREAKFAST

John Zetts, WL/MLPO, Chair

8:00-8:30am:

SPACE COMMUNICATIONS

Carl Gass, PL/VTRA

8:30-9:00am:

IMAGE PROCESSING

Charles Woods, RL/EROP

9:00-9:30am:

SYNTHESIS AND CHARACTERIZATION OF 2-PHOTON RESONANT

THIRD-ORDER NLO MATERIALS

Bruce A. Reinhardt, WL/MLBP

9:30-:950am:

SYNTHESIS OF 2ND-ORDER NLO CHROMOPHORES AND POLYMERS

FOR EO APPLICATIONS Bruce A. Reinhardt, WL/MLBP

9:50-10:10am:

BREAK

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APPENDIX K

ANNUAL REPORT

CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM CONTRACT NO. F49620-95-C-0026

Period of Performance: 3/1/96 - 2/28/97

Prepared For:

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH CHEMISTRY AND LIFE SCIENCES DIRECTORATE

Dr. Genevieve Haddad, Program Manager

Presented By:

UES, Inc. 4401 Dayton-Xenia Road Dayton, OH 45432-1894

INTRODUCTION

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition), Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology, Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The first option year included: 103 Proposals that were reviewed; 3 Program/Contractor Reviews; 2 Workshops and 4 Panel Meetings.

A. Evaluations of Individual Research Proposals

UES sent out 103 proposals to 373 evaluators during the performance period of 1 March 1996 through 28 February 1997.

UES has been providing the Directorate of Chemistry and Life Sciences a Summary of Proposals Under Review (SPUR) report on a biweekly basis. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the Program Managers to have a current listing of all proposal activity.

B. <u>Contractor/Program Reviews</u>

A total of 3 program reviews were held during this contract year.

1. The first program review was joint and entitled Molecular Dynamics (MD) and High Energy Density Matter (HEDM). It was held 2-7 June 1996 at the University of Colorado in Boulder, CO. Of the 120 attendees, 52 were speakers. The HEDM Program is designed to search for new energetic forms of matter with possible future applications to Air Force propulsion and energy storage systems. Recent advances

and accomplishments of the program were outlined at this meeting. In addition, a workshop was held on the interactions between theory and syntheses. UES acquired the meeting site and made all arrangements for the meeting including meals and audio visual equipment. UES also provided on site support.

Dr. Michael Berman, Program Manager

2. The second program review was in the area of **Toxicology** and was held 12-13 December 1996 at the Holiday Inn I-675 in Fairborn, OH. The purpose of this meeting was to review basic research in toxicology which is supported by or of interest to the AFOSR program in Toxicology. Each participant presented a 25 minute presentation discussing the primary objectives, results and conclusions of past research, emphasizing major accomplishments, and indicating new directions and areas of future research. The review strived to achieve several goals: to inform each participant of other work being conducted under the AFOSR Toxicology Program; to exchange scientific information; to foster collaboration; and to generate new ideas. In addition, AFOSR acquired information to facilitate technology transfers, Air Force justification of research efforts, and decision-making with respect to programmatic organization. Of the 19 in attendance, 16 were speakers. UES acquired the meeting site; made all arrangements for the meeting including meals and audio visual equipment.

Dr. Walter Kozumbo, Program Manager

3. The third program review entitled **New World Vista Coordination Meeting** was held 25 February 1997 at the Holiday Inn in Pasadena, CA. The purpose of the coordination meeting was to review the polymer related approved in-house tasks in the New World Vista. Topics included Global Mobility Composites, Light Weight Structural Materials for Space, Deployable Antenna Membranes, Uninhibited Aerial Vehicles and Light Weight Antenna Structures. There were eleven in attendance. UES acquired the meeting site; made all arrangements for the meeting including breaks and audio visual equipment.

Dr. Charles Lee, Program Manager

C. Workshops

Two workshops were held during this year's effort.

1. A **DALM** (**Diazoluminomelanin**) **Workshop** was held on 3-5 March 1996 at the North Redington Beach Hilton Hotel in North Redington Beach, Florida. There were 27 in attendance of which 15 were speakers. The purpose of this meeting was to review the research that has been conducted in relationship to a recently discovered slow-luminescent compound called diazoluminomelanin (DALM). Since its discovery, this compound has demonstrated rather unique properties, some of which have already been exploited to produce applications related to the fields of medicine, radiation, dosimetry, and hazardous waste remediation. Another potential application for DALM is in the area of infrared sensor development. This application was addressed and included some of the planned research on infrared sensors in biological systems. Unless we acquire a

fundamental understanding of DALM, its structure and synthesis as well as its physical, chemical and biological properties, further applications-oriented progress will be slowed. Our purpose was to review what is known about the chemistry, physics and biology of DALM and its potential applications so that we may be in a better position to make good decisions concerning future basic research endeavors in this area. UES provided travel, per diem and honorarium for six advisors; acquired the meeting site; made all arrangements for the meeting including meals and audio visual equipment. In addition UES provided on site support.

Dr. Walter Kozumbo, Program Manager

2. A workshop on **DOD** Chemistry was held 18-20 September 1996 at the Fort Magruder Inn and Conference Center, Williamsburg, VA. UES acquired the meeting site and made arrangements for the meeting including audio visual equipment. Dr. Michael Berman, Program Manager

D. Panel Meetings

Four panel meetings were held during this year's effort.

1. A panel meeting was held on **Organic Thin Film for Optical Applications** at the Hyatt Regency O'Hare Hotel, Rosemont, Illinois on 9 April 1996. UES provided travel and per diem for 3 advisors in attendance as well as the meeting location and refreshments.

Dr. Charles Lee, Program Manager

2. A panel meeting was held on **Molecular Dynamics and Theoretical**Chemistry at the Hyatt Regency O'Hare Hotel, Rosemont, Illinois on 2 May 1996.
Seven advisors reviewed proposals in the mentioned area. UES made arrangements for the meeting location. UES also provided travel, per diem and honorarium to the advisors.
Reviews were secured from six outside reviewers.

Dr. Michael Berman, Program Manager

- 3. A panel meeting was held on **High Energy Density Matter** in conjunction with the Program Review on 8 June 1996 at the University of Colorado. UES made arrangements for the meeting location as well as provided travel, per diem and honorarium for three panel members. Outside reviews were secured from six reviewers. Dr. Michael Berman, Program Manager
- 4. A second **Molecular Dynamics and Theoretical Chemistry** panel meeting was held at the Courtyard by Marriott O'Hare in Des Plaines, IL on 3 October 1996. Seven advisors reviewed proposals in the mentioned area. UES made arrangements for the meeting location. UES also provided travel, per diem and honorarium to the advisors. Reviews were secured from sixteen outside reviewers.

Dr. Michael Berman, Program Manager

E. Advisors

In addition to advisors provided for Program Reviews, Workshops and Panel Meetings, UES provided travel, per diem and in many cases, honorarium for the following advisors:

David H. Cohen, Neuroscience for the DOD Evaluation of Basic Research Programs Meeting, Institute for Defense Analysis, Arlington, VA, 22-26 April 1996

James Todd, Visual Perception of 3-D, Air Force Armstrong Laboratory, WPAFB, OH, 4-6 June 1996.

Michael Tarr, Representations of Shape in Object Recognition, Air Force Armstrong Laboratory, WPAFB, OH, 4-6 June 1996.

Charles Czeisler, PRET Meeting, Sam Technologies, San Francisco, CA, 31 July 1996 and Boeing Commercial Aviation, Seattle, WA, 1 August 1996.

Subhash Basak, Computational Toxicology to evaluate and advise the AFOSR Predictive Toxicology Program in the area of mathematical modeling, WPAFB, OH, 5-7 August 1996.

Irving Biederman, Human Pattern Recognition, Air Force Phillips Laboratory, Kirtland AFB, NM, 19 October 1996.

Joseph Goldberg and Stephen Hess, Cognitive Workload, Air Force Armstrong Laboratory, Brooks AFB, TX and WPAFB, OH, 31 October and 1 November 1996.

Marcel Adam Just and Javier Lerch, Integrated Assessment of Workload in Decision-Making, Air Force Armstrong Laboratory, Brooks AFB, TX and WPAFB, OH, 18 November 1996.

Bob Pozos, Deborah a. Boehm-Davis, Wayne Gray and Len Adelman, Understanding and Measuring Cognitive Workload, Air Force Armstrong Laboratory, Brooks AFB, TX and WPAFB, OH, 20-26 November 1996.

Gavriel Salvendy and Robert W. Proctor, Measurement of Cognitive Workload, Air Force Armstrong Laboratory, WPAFB, OH, December 1996.

Bellina Veronesi and Susan Leeman, JP-8 Jet Fuel Toxicity, University of Arizona, Tucson, AZ, 13-14 February 1997.

SUMMARY

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Dr. Julien M. Christensen, Program Manager, Judith M. Flory, Program Administrator, Betty Kerans, Program Assistant, and Donna Tinley, Assistant Program Administrator. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

LIST OF APPENDICES

Breakdown of Research Proposals by Program Manager

Program for Molecular Dynamics Contractor's Meeting, University of Colorado, Boulder, Colorado, 2-5 June 1996

Program for **High Energy Density Matter Contractor's Meeting**, University of Colorado, Boulder, Colorado, 5-7 June 1996

Program for **Toxicology Program Review**, Holiday Inn Conference Center, Fairborn, Ohio, 12-13 December 1996

Program for New World Vista Meeting, Pasadena Holiday Inn, Pasadena, California, 25 February 1997

Program for **Workshop on DALM (Diazoluminomelanin)**, North Redington Beach Hilton Resort, North Redington Beach, Florida, 3-5 March 1996

Summary of Reviews, Molecular Dynamics and Theoretical Chemistry Panel Meeting, Hyatt Regency O'Hare Hotel, Rosemont, Illinois, 2 May 1996

Summary of Reviews, **High Energy Density Matter Panel Meeting**, University of Colorado, Boulder, Colorado, 8 June 1996

Summary of Reviews, Molecular Dynamics and Theoretical Chemistry Panel Meeting, Courtyard by Marriott O'Hare, Des Plaines, Illinois, 3 October 1996

BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER

PROGRAM MANAGER	NO. OF PROPOSALS	
** 11 1	10	
Haddad	10	
Tangney	20	
Lee	25	
Kozumbo	14	
Kroll	1	
De Long	4	
Hedberg	1	
Berman	22	
Roach	6	

1996 Molecular Dynamics Contractors Meeting University of Colorado, Boulder, Colorado 2-5 June 1996

Sunday, 2 June 1996

6:00 - 7:00	Registration
7:00 - 9:30	Poster Session, Reception

Monday, 3 June 1996

Monday, 5 suite 1990		
8:15 - 8:30	Introductory Remarks, Dr. Michael Berman, AFOSR	
8:30 - 9:00	Time Resolved Dynamics In Molecular Cluster Ions Dr. W. Carl Lineberger, University of Colorado	
9:00 - 9:30	Stimulated Raman Pumping and Electron Detachment Dynamics of Carbon Cluster Anions Dr. Daniel M. Neumark, University of California	
9:30 - 10:00	The Effective Fragment Method for Solvation Dr. Mark S. Gordon, Iowa State University	
10:00 - 10:30	Break	
10:30 - 11:00	Chemistry in the Spacecraft Environment Dr. Rainer A. Dressler, Phillips Laboratory	
11:00 - 11:30	Potential Energy Surfaces for Some Gas Phase Reactions Dr. Keiji Morokuma, Emory University	
11:30 - 12:00	Does Air Burn? or The Dynamics of Chemical Reactions Under Extreme Conditions Dr. Raphael D. Levine, The Hebrew University of Jerusalem	
12:00 - 1:30	Lunch	
1:30 - 2:00	Conformations of Macromolecules in the Gas Phase Dr. Michael T. Bowers, University of California	

Monday, 3 June 1996 (cont'd)

2:00 - 2:30	Ion Rotational Distributions at Near-Threshold Photoelectron Energies Dr. Vincent McKoy, California Institute of Technology
2:30 - 3:00	Reactive Scattering of Hyperthermal, State-Selected Molecular Ions on Surfaces Dr. Dennis C. Jacobs, University of Notre Dame
3:00 - 3:30	Break
3:30 - 4:00	Reactive Processes in Molecule-Surface Collisions Dr. Curt Wittig, University of Southern California
4:00 - 4:30	Kinetic Simulations of Island Formation During Epitaxial Deposition Prof Horia Metiu, University of California
4:30 - 5:00	Dynamics of Fracture in Nanophase Silicon Nitride: Million Atom Molecular-Dynamics Simulations on Parallel Machines Dr. Rajiv K. Kalia, Louisiana State University

Tuesday, 4 June 1996

8:30 - 9:00	Recent Progress in Studies of Femtosecond Dynamics and Control of Reactions Dr. Ahmed Zewail, California Institute of Technology
9:00 - 9:30	Fluctuations and Relative Stability in Systems Far From Equilibrium Dr. John Ross, Stanford University
9:30 - 10:00	Vibrational Dynamics of Polyatomic Molecules in Polyatomic Supercritical Fluids and Liquids Dr. Michael D. Fayer, Stanford University
10:00 - 10:30	Break
10:30 - 11:00	Thermal Energy Reactions of Mass Selected Cluster Ions Dr. Al A. Viggiano
11:00 - 11:30	State Resolved Dynamics of Ion-Molecule Processes Dr. Stephen R. Leone, University of Colorado
11:30 - 11:45	Break
11:45 - 12:00	Dr. Michael Berman, AFOSR
12:00 - 2:00	Lunch
2:00 -	Informal Discussions
7:30 - 8:00	Met-Cars: Optical Excitation and Dynamics of Ionization Dr. A. Welford Castleman, Jr., The Pennsylvania State University
8:00 - 8:30	Photodissociation and Photoionization of Metal Compound Clusters Dr. Michael A. Duncan, University of Georgia
8:30 - 9:00	Density Functional Theory for Large Molecules and Application to Metcars Dr. Gustavo E. Scuseria

Wednesday, 5 June 1996

8:30 - 9:00	Dynamics of Rotational and Vibrational non-Equilibrium in Thermospheric Species Dr. William A. M. Blumberg, Phillips Laboratory
9:00 - 9:30	Inelastic and Reactive Collision Dynamics of Atmospheric Species via High Resolution IR Lasers Dr. David J. Nesbitt, University of Colorado
9:30 - 10:00	Time- and State-Resolved Dynamics of O-Atom Reactions Dr. Michael Casassa, National Institute of Standards and Technology
10:00 - 10:30	The Collisional Coupling of the Highly Excited $a^{11}\sum_{u}$, $a^{1}\Pi_{g}$, and $w^{1}\Delta_{u}$ Electronic States of Nitrogen Dr. Daniel H. Katayama, Phillips Laboratory
10:30 - 11:00	Break
11:00 - 11:30	HCP↔HPC Isomerization, Spectral Unzipping, and Triplet States of Acetylene Dr. Robert W. Field, Massachusetts Institute of Technology
11:30 - 12:00	Internal Energy in Reaction Dynamics Dr. F. Fleming Crim, University of Wisconsin - Madison
12:00 - 12:30	PUMP-DUMP-PROBE in Crossed and Uncrossed Molecular Beams Dr. Alec M. Wodtke, University of Southern California, Santa Barbara
12:30 - 1:00	Is Density Functional Theory Appropriate for Inorganic Molecular Anions? Dr. Henry F. Schaefer, III
Afternoon	BBQ at Flagstaff Mt. (Joint with HEDM Meeting)

1996 High Energy Density Matter Contractors Meeting University of Colorado, Boulder, Colorado 5-7 June 1996

Wednesday, 5 June 1996

Afternoon	BBQ at Flagstaff Mt. (Joint with Molecular Dynamics)
6:00 - 7:00	Registration
7:00 - 9:30	HEDM Poster Session
Thursday, 6 June 19	996
8:30 - 8:45	Introductory Remarks, Dr. Michael Berman, AFOSR
8:45 - 9:00	Phillips Laboratory Remarks Dr. Pat Carrick, Phillips Laboratory
9:00 - 9:15	Phillips Laboratory Remarks Dr. Stephen L. Rodgers, Phillips Laboratory
9:15 - 9:30	Break
9:30 - 10:00	Solid Hydrogens Doped with Atomic and Molecular Oxygen Dr. V. Ara Apkarian, University of California
10:00 - 10:30	Mass Spectrometry Studies of Pick Up by Helium Clusters Dr. Ken Janda, University of California
10:30 - 11:00	Calorimetric Measurements of O Atom Concentration in a Solid Ar Matrix Dr. Peter Taborek, University of California, Irvine
11:00 - 11:30	Status Report of Cryogenic Solid Hybrid Rocket Engine Development for HEDM Demonstrations Dr. Eric Rice, Orbitec, Inc.
11:30 - 12:45	Lunch
12:45 - 1:15	Progress Towards Depositions of Velocity Selected Aluminum Atoms into Cryogenic para-Hydrogen Matrices Dr. Mario E. Fajardo, Phillips Laboratory

Thursday, 6 June 1996 (cont'd)

1:15 - 1:45	Spectral Theory of Physical and Chemical Binding in HEDM Systems Dr. Jeffrey A. Sheehy, Phillips Laboratory
1:45 - 2:15	Quantum Molecular Dynamics Simulations of Low Temperature Hydrogen Systems Dr. Gregory A. Voth, University of Pennsylvania
2:15 - 2:45	The Interaction of Alkali Atoms with Large Clusters of n-H ₂ , p-H ₂ and p-D ₂ Probed by Laser Spectroscopy Dr. Giacinto Scoles, Princeton University
2:45 - 3:00	Break
3:00 - 3:30	Resonant Photoionization Spectroscopy of A1(Ar) _n Clusters Dr. Mitchio Okumura, California Institute of Technology
3:30 - 4:00	Spectroscopic Characterization of Non-Bonding Interactions of the Boron Atom Dr. Paul J. Dagdigian,, The Johns Hopkins University
4:00 - 4:30	Structure and Energetics of $B(Ar)_n$ and $B(N_2)$ Clusters Dr. Millard H. Alexander, University of Maryland
7:30	Theory/Synthesis Workshop

Friday, 7 June 1996

8:15 - 8:45	Cryogenic Solid Combustion Dr. William Larson, Phillips Laboratory
8:45 - 9:15	Generation of Energetic Species in Solid Oxygen with Tunable Ultraviolet Light Dr. Richard A. Copeland, SRI International
9:15 - 9:45	The Overtone $Q_v(0)$ Transitions in Hydrogen Dr. Takeshi Oka, The University of Chicago
9:45 - 10:15	Search for Metallic Hydrogen in the Extended Infrared Dr. Isaac F. Silvera, Harvard University
10:15 - 10:45	Break
10:45 - 11:15	Reactions of Laser-Ablated Boron Atoms with NH ₃ , CH ₃ NH ₂ and NO to Form Novel Boron Insertion Products Dr. Lester Andrews, University of Virginia
11:15 - 11:45	Excited States for Molecules an Clusters Dr. Rodney J. Bartlett, University of Florida
11:45 - 12:15	Nonadiabatic Processes Affecting Detection and Preparation of Energetic Materials Dr. David R. Yarkony, Johns Hopkins University
12:15 - 12:45	Potential Energy Surfaces and Dynamics for High Energy Species Dr. Mark S. Gordon, Iowa State University
12:45 - 2:00	Lunch
2:00 - 2:30	Discussion
2:30 - 3:00	Quantum Mechanical Study of the Energetics of C ₈ H ₈ Hydrocarbons Dr. E. J. Wucherer, Phillips Laboratory
3:00 - 3:30	Synthesis of High-Energy Density Materials Based on Strained-Ring Compounds Dr. William P. Dailey, University of Pennsylvania
3:30 - 3:45	Break

Friday, 7 June 1996 (cont'd)

3:45 - 4:15	Recent Progress in the Theory and Synthesis of Novel High Energy Density Materials Dr. Karl O. Christe, Hughes STX and Propulsion Science Division
4:15 - 4:45	Extra-High Energy Oxidizers and Fuels Dr. Robert J. Schmitt, SRI International
4:45 - 5:00	Closing Remarks, adjournment



1000-1015 COFFEE BREAK

AFOSR TOXICOLOGY PROGRAM REVIEW

Holiday Inn Conference Center Fairborn, Ohio 12 - 13 December 1996

Wednesday, 11 December 1996

1700-1830	REGISTRATION
1830-2000	Evening Reception at Holiday Inn
	Thursday, 12 December 1996
Introductory	Comments
0730-0830	REGISTRATION AND CONTINENTAL BREAKFAST
0830-0845	AFOSR'S Toxicology Program Dr. Walt Kozumbo, AFOSR, Bolling AFB, DC
Toxicology Program at Armstrong Laboratory/Tri-Service Toxicology	
0845-0900	Air Force Laboratory Toxicology Programs Dr. John M. Frazier, Armstrong Laboratory, WPAFB
0900-0915	Trichlorethylene - Metabolic Pathway Modeling Dr. Jeff Fisher, Armstrong Laboratory, WPAFB
0915-0930	Halon Replacements Dr. Allen Vinegar, ManTech at WPAFB
0930-0945	Dermal Penetration Dr. James N. McDougal, Geo-Centers at WPAFB
0945-1000	Total Petroleum Hydrocarbons Captain Wade H. Weisman, Armstrong Laboratory, WPAFB

In Vivo Toxic Effects/Biomarkers

1015-1045	The Role of Substance P in a Model of Chronic Exposure to JP-8 Jet Fuel Mark L. Witten, University of Arizona
1045-1115	Immunotoxicology of JP-8 Jet Fuel Exposure David T. Harris, University of Arizona
1115-1145	Detoxication Enzymes as Biomarkers of Toxin Exposure Drs. Frank L. Siegel & Steven E. Kornguth, University of Wisconsin
1145-1215	NMR Studies of Liver Metabolism Following Exposure to Trichloroacetate and Other Peroxisome Proliferators Dr. Nicholas V. Reo, Wright State University
1215-1330	LUNCHEON at Holiday Inn
1330-1400	Biomarker Analysis of Human Breath for Early Prediction of Hepatoxocity Dr. Terence H. Risby, Johns Hopkins University
1400-1430	Changes in Steroid Hormone Metabolism as Noninvasive Biomarkers of Toxicant Exposure and Effect Dr. Gerald A. LeBlanc, North Carolina State University
Mechanistica	ally Based Toxicology
1430-1500	Mechanisms Associated With the Toxicity of Naphthalene, Chromium and Cadmium Dr. Sidney J. Stohs, Creighton University
1500-1515	COFFEE BREAK
1515-1530	Perfluorinated Fatty Acids of Specific Chain Lengths Directly Inhibit Gap Jumctional Intercellular Communication and Indirectly Inhibit via H ₂ O ₂ in Glutathione-Sufficient But Not Glutathione-Deficient Cells Dr. Brad L. Upham, Michigan State University
1530-1600	Chromium Toxicity: Reductive Enzymes in Humans Dr. Charles R. Myers, Medical College of Wisconsin
1600-1630	Depletion of Nuclear Poly (ADP-ribose) Polymerase by Antisense RNA Expression: Influences on DNA Repair and Replication, and Survival of Cells to Genotoxic Agents. New Studies on Apoptosis. Dr. Mark E. Smulson, Georgetown University
1630-	Discussion and adjournment until tomorrow morning.

Friday, 13 December 1996

CONTINENTAL BREAKFAST at Holiday Inn 0730-0830 Predictive Toxicology: Alternatives to Animal Use in Toxicity Assessment An Interdisciplinary and Alternative Approach to Assess Carcinogenicity of 0830-0900 Chlorobenzenes Dr. Raymond S.H. Yang, Colorado State University Predictive Toxicology 0900-0930 Dr. John M. Frazier, Armstrong Laboratory, WPAFB Corneal Equivalents for In Vitro Testing of Ocular Irritants 0930-1000 Dr. Thomas E. Eurell, University of Illinois **COFFEE BREAK** 1000-1015 Protein Biomarkers of Chemical Exposure and Molecular Toxicology 1015-1045 Dr. Frank A. Witzmann, Indiana University-Purdue University at Indianapolis Development of QMSA and QSAR Methods for Hazard Assessment of 1045-1115 Chemicals: Tools for Computational Toxicology Dr. Subhash C. Basak, University of Minnesota Open discussion and concluding remarks. 1115-1200

New World Vista Meeting February 25, 1997

Pasadena Holiday Inn Hotel (Room #)

8:00 8:30 9:00 9:30 1000	Breakfast Opening Remarks (Overview of NWV) Discission Session Scott Wierschke (Polymers in Rocket Applications) Break
	(Low Cost, Light Weight Membrane Structure - Antenna)
1030	Jonathan Bishop - PL
1100	(Family of Unmanned Aerial Vehicle)
1120	Dave Curliss (WL) (Air Mobility - Composites)
1140	Frances Abrams (Carbon Foams)
1200	Lunch
	(Light Weight Structure and Materials in Space)
1300	Steve Rogers/ Wade Adams (PL/ML)
1310	Kevin Chaffee - PL
1000	Polymer Innovation for Rocket Propulsion
1330	Richard Vaia - (WL) Advanced Light Weight Materials
1350	Charles Stein (PL) Synergism in the Interaction of Atomic Oxygen, Electrons, and UV Radiation with Organic Polymers
1410	Wes Hoffman (PL) Light Weight, Low Cost Rocket Propulsion Manufacturing Technology
1430	Alok Das (PL)
	Theoretical and Experimental Studies of Vibronacoustic Systems
1440	Break
1500	Closed Session (Government Only)



AFOSR Workshop on DALM (Diazoluminomelanin) North Redington Beach Hilton Resort, North Redington Beach, FL 3-5 March 1996

Sunday, 3 March 1996

1700-1830 1830-2030	REGISTRATION (The Verandah adjacent to hotel restaurant) Evening Reception at North Redington Beach Hilton Resort (The Verandah) Monday, 4 March 1996
Introduction	
0730-0800	REGISTRATION AND CONTINENTAL BREAKFAST (Conference Rooms C & D)
0800-0810	Welcome and Meeting Objectives Dr. Walt Kozumbo, AFOSR, Bolling AFB, DC
0810-0830	Historical Perspective and Potential Importance of DALM Dr. Johnathan Kiel, Armstrong Lab., Brooks AFB, TX
Properties, Structure and Synthesis of DALM (Dr. Kiel as Moderator)	
0830-0900	Organic Synthesis of DALM Mr. Gerald O'Brien, SAIC, San Antonio, TX
0900-0930	Instrumentation for Real Time Measurement of DALM Luminescence Mr. Brion Burghard, Pacific Northwest National Labs., Richland, WA
0930-1000	Chemical Structure of DALM Based on NMR Dr. John Wright, Southeastern Oklahoma State Univ., Durant, OK
1000-1015	COFFEE BREAK
1015-1045	Biosynthesis of DALM TSgt. John L. Alls, Armstrong Lab., Brooks AFB, TX
1045-1115	Molecular Biology of DALM Biosynthesis Dr. Jill E. Parker, Armstrong Lab., Brooks AFB, TX

1115-1145	Purification & Characterization of <u>Bacillus Anthracis</u> Aerobic Nitrate Reductase (Dalm Synthase) Lt. Col. Larry D. Strawser, US Air Force Academy, Colorado Springs, CO
1145-1200	Discussion
1200-1330	LUNCH (The Verandah)
1330-1400	Biosynthesis of DALM in HL-60 Cells and Other Attempts of Eukaryotic Cell Biosynthesis Dr. John G. Bruno, Applied Research Assoc., Tyndall AFB, FL
	Dr. John G. Bruno, Applied Research Assoc., Tyndan Arb, FL
1400-1430	Molecular Modeling and the Discovery of the Solid State Properties of DALM Maj. Eric A. Holwitt, Armstrong Lab., Brooks AFB, TX
Potential Applications of DALM (Maj. Eric A. Holwitt as Moderator)	
1430-1500	Requirement for New RFR Dosimetric Techniques Using DALM Dr. Johnathan L. Kiel, Armstrong Lab., Brooks AFB, TX
1500-1530	DALM and Other Poly-Monohydroxyarylamino Acids as Antibiotics Dr. Johnathan L. Kiel, Armstrong Lab., Brooks AFB, TX
1530-1545	COFFEE BREAK
1545-1600	Metallo-DALM Complexes as Catalysts for Hydrazine Breakdown Maj. Eric A. Holwitt, Armstrong Lab., Brooks AFB, TX
1600-1630	The SERDP Project: Metallo-DALM for the Remediation of Hydrazines Lt. David J. Kuch, Armstrong Lab., Tyndall AFB, FL
1630-1700	Discussion
1700	Adjournment until tomorrow morning
Tuesday, 5 March 1996	
0730-0830	CONTINENTAL BREAKFAST (Conference Rooms C & D)
Role of DALM in the AFOSR Biomimetic Infrared Sensor Initiative	
0830-0900	DALM as a Photoreactive Material and Its Use in IR Sensors Dr. Thomas Cooper, Wright Lab., Wright-Patterson AFB, OH Dr. John Taboada, Armstrong Lab., Brooks AFB, TX

0900-0930	Infrared Sensing in Pit Vipers Dr. Richard C. Goris, Yokohama City University, Yokohama, Japan
0930-1000	Infrared Sensing in Boids Dr. Michael S. Grace, University of VA., Charlottesville, VA
1000-1015	COFFEE BREAK
1015-1045	Infrared Sensing in Single-Cell Organelles Dr. Guenter Albrecht-Buehler, Northwestern Univ., Chicago, IL
1045-1100	Discussion and adjournment
1100-1300	LUNCH (on your own) Meeting of Reviewers and Program Managers at Hotel

SUMMARY OF REVIEWS Molecular Dynamics Panel Meeting

Partitioning and Reactivity of Environmental Solutes in Multiphase Systems
- Donald G. Truhlar, University of Minnesota

Steven D. Colson, Pacific Northwest Laboratory ()

Jeff Hay, Los Alamos National Laboratory (A/1)

George Schatz, Northwestern University (A/3)

Ann B. McCoy, Ohio State University (A/3)

96-NL-131 Atomic Scale Chemistry and Structure of Ceramic/Metal Interfaces
- David N. Seidman, Northwestern University

Steven D. Colson, Pacific Northwest Laboratories (
)
Jeff Hay, Los Alamos National Laboratory (A-/2)
J. Michael White, University of Texas (A-/3)
David Vanderbilt, Rutgers University (A-/4)

96-NL-135 Physical Chemistry of Energetic Nitrogen Compounds
- Robert D. Coombe, University of Denver

Laurie J. Butler, University of Chicago (A-/B+/2/-4/5)
Charles Parmenter, Indiana University (A-/3>4)
James Weisshaar, University of Denver (A/4)
J. Michael White, University of Texas (A/1)
David Benard, Rockwell Science Center (A/1)

96-NL-136 Spectroscopy of Anions and Transition States Using Stimulated Raman Pumping

- Daniel M. Neumark, University of California

Charles Parmenter, Indiana University (A/3)
George Schatz, Northwestern University (A+/1)
James Weisshaar, University of Denver (A/1)

Theoretical Methods for Optimal Design of Biomaterials: 96-NI-137 **Energy Landscape Perspective**

Devarajan Thirumalai, University of Maryland

Jeff Hay, University of Maryland (B+/2) George Schatz, Northwestern University (B/3)

Bruce Garrett, Pacific Northwest Laboratory (A/A-/2)

Kenneth Jordan. University of Pittsburgh (A/4)

Triplet States of Small Molecules: Photochemistry, Spectroscopy, and 96-NI_138 **Dynamics**

- Robert W. Field, Massachusetts Institute of Technology

Laurie J. Butler, University of Chicago (A/2)

Steven D. Colson, Pacific Northwest Laboratory ()

Charles Parmenter, Indiana University (A/2)

James Weisshaar, University of Wisconsin (A+/2)

Clusters of Transition Metal Compounds: Building Blocks of New Materials 96-NI_140

- Albert Welford Castleman, Jr., Pennsylvania State University

Laurie J. Butler, University of Chicago (A/A-/3)

Steven D. Colson, Pacific Northwest Laboratory ()

Charles Parmenter, Indiana University (A/3)

James Weisshaar, University of Wisconsin (B+/2).

I. Michael White. University of Texas (A+/2)

Optimization of Geometric Structures of New Materials on Parallel 96-NL-148

Computers

- John H. Weare, University of California

Jeff Hay, Los Alamos National Laboratory (A/2)

George Schatz, Northwestern University (B+/2)

J. Michael White, University of Texas (-/4)

Albert F. Wagner, Argonne National Laboratory (A-/B+/2)

SUMMARY OF REVIEWS High Energy Density Matter Panel Meeting

96-NL-133 Reactions of Laser-Ablated Metal Atoms to Produce High Energy Molecules

- Lester Andrews, University of Virginia

Vladimir E. Bondybey, Technical University of Munich (A-/1)

Bruce C. Garrett, Pacific Northwest National Laboratory (A/3)

Clark W. Hawk, UAH Propulsion Research Center (B+/5)

Lon B. Knight, Furman University (A+/2)

James J. Valentini, Columbia University (A/2)

John S. Winn, Dartmouth College (A/2)

Derek M. Lindsay, City University of New York, City College (A/2)

96-NL-147 Spectroscopy of Metal Atoms Trapped in Solid Helium

- Ken G. Libbrecht, California Institute of Technology

Vladimir E. Bondybey, Technical University of Munich (B+/1)
Bruce C. Garrett, Pacific Northwest National Laboratory (A-/B+/3)
Clark W. Hawk, UAH Propulsion Research Center (A/5)
Marilyn Jacox, National Institute of Standards & Technlogy (B+/1)
Derek M. Lindsay, City University of New York, City College(B+/2)
James J. Valentini, Columbia University (B/2)

96-NL-153 Spectroscopic and Dynamical Studies of Impurities in Solid Hydrogen: A Possible Road to HEDM

-Takeshi Oka, The University of Chicago

Vladimir E. Bondybey, Technical University of Munich (A+/1)
Bruce C. Garrett, Pacific Northwest National Laboratory (A+/3)
Clark W. Hawk, UAH Propulsion Research Center (B/5)
Terry A. Miller, Ohio State University (A/3)
James J. Valentini, Cohumbia University (A-/2)
John S. Winn, Dartmouth College (A/1)

SUMMARY OF REVIEWS AFOSR Molecular Dynamics/Theoretical Chemistry Review Panel

96-NL-190 Femtosecond Shock Wave Dynamics of Insensitive Energetic Materials
- Dana D. Dlott, University of Illinois

Thomas B. Brill, University of Delaware (A/3)

Laurie J. Butler, University of Chicago (A-/B+/4/5)

Charles S. Parmenter, Indiana University (A/3)

James C. Weisshaar, University of Wisconsin ((A/4))

J. Michael White, University of Texas at Austin (A+/1)

96-NL-201 State-Resolved Thermal/Hyperthermal Collision Dynamics of Atmospheric Species

- David J. Nesbitt (University of Colorado)

Laurie J. Butler, University of Chicago (A/2)

Paul L. Houston, Cornell University (A/1)

Charles S. Parmenter, Indiana University (A-/2)

James C. Weisshaar, University of Wisconsin (A+/2)

96-NL-202 Ultrafast Nonlinear Optical Investigations of Subcritical Fluids
- Michael D. Fayer, Stanford University

Joan F. Brennecke, University of Notre Dame (A-/2)

Laurie J. Butler, University of Chicago (A-/4)

Charles S. Parmenter, Indiana University (A-/3)

Theodore W. Randolph, University of Colorado (A-/2)

George Schatz, Northwestern University (A/3)

I Michael White. University of Texas at Austin (A/2)

96-NL-205 Chemistry Under Extreme Conditions

- James L. Kinsey, Rice University

Charles S. Parmenter, Indiana University (B+/4)

Lawrence R. Pratt, Los Alamos National Laboratory (A/4-5)

George Schatz, Northwestern University (A/2)

John Tully, Yale University (A+/1)

96-NL-208 A New Method for Fast and Accurate Atomic-Scale Simulation of Materials and Its Application to Thin-Film Epitaxy

- Kristen Fichthorn, Pennsylvania State University

Lawrence R. Pratt, Los Alamos National Laboratory (B/1)

Lionel M. Raff, Oklahoma State University (B+/2)

George Schatz, Northwestern University (A-/2)

Arthur F. Voter, Los Alamos National Laboratory (B+/A//1)

J. Michael White, University of Texas at Austin (B+/1)

96-NL-209 Dynamics of Metal Species of Atmospheric Importance

- John Lombardi, City College of City University of New York

Steven D. Colson, Pacific Northwest National Laboratory (A-/2)

Michael D. Morse, University of Utah (A-/B+/2)

James C. Weisshaar, University of Wisconsin (C/1)

J. Michael White, University of Texas at Austin (B+/2)

96-NL-210 Development and Applications of Quantum Molecular Solvation Theory

Reactions in Solutions

- Thanh N. Truong, University of Utah

Jiali Gao, State University of New York at Buffalo (A-/1)

Lawrence R. Pratt. Los Alamos National Laboratory (B+/1)

George Schatz, Northwestern University (A-/B+/3)

Walter Stevens, National Inst. of Standards & Technology (B+/4)

96-NL-211 Structure and Dynamics of Metal-Containing Clusters

- Michael A. Duncan, University of Georgia

Peter B. Armentrout, University of Utah (A/1)

Laurie J. Butler, University of Chicago (A/3)

Steven D. Colson, Pacific Northwest National Laboratory (A+/1)

James C. Weisshaar, University of Wisconsin (A-/1)

96-NL-213 Theoretical Determination of Optimized Structures for Molecular

Complexes and Clusters

-Peter Pulay, University of Arkansas

Frank Jensen, Odense University, Denmark (A/1)

Lawrence R. Pratt. Los Alamos National Laboratory (A/4-5)

George Schatz, Northwestern University (A-/2)

Michael C. Zerner, University of Florida (A+/1)

96-NL-214 A Fundamental Investigation of Metal/Ceramic Interfaces: Toward Nanostructure Control

- Randall Boehm, New Mexico Highlands University

Steven D. Colson, Pacific Northwest National Laboratory (B+/4)
David A. Dixon, Pacific Northwest National Laboratory (C/1)
Theodore E. Madey, Rutgers University (B/2)

I. Michael White, University of Texas at Austin (B-/2)
(A for the problem, C for the method)

96-NL-219 Pulsed Field Ionization Spectroscopy of Mesospheric Molecules:
Elucidating the Chemistry of Metal Atoms in the Upper Atmosphere
- Mitchio Okumura, California Institute of Technology

Kit H. Bowen, Jr., Johns Hopkins University (A+/2)
Laurie J. Butler, University of Chicago (A/A-/3)
Steven D. Colson, Pacific Northwest National Laboratory (A/1)
Charles S. Parmenter, Indiana University (A-/B+/3)
James C. Weisshaar, University of Wisconsin (A-/2)

APPENDIX L

ANNUAL REPORT

CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM CONTRACT NO. F49620-95-C-0026

Period of Performance: 3/1/97 - 2/28/98

Prepared For:

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH CHEMISTRY AND LIFE SCIENCES DIRECTORATE

Dr. Genevieve Haddad, Program Manager

Presented By:

UES, Inc. 4401 Dayton-Xenia Road Dayton, OH 45432-1894

INTRODUCTION

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology, Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The second option year included: 138 Proposals that were reviewed; 7 Program/Contractor Reviews; 3 Workshops and 4 Panel Meetings.

A. Evaluations of Individual Research Proposals

UES sent out 138 proposals to 422 evaluators during the performance period of 1 March 1997 through 28 February 1998.

UES has been providing the Directorate of Chemistry and Life Sciences a Summary of Proposals Under Review (SPUR) report on a biweekly basis. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the Program Managers to have a current listing of all proposal activity.

B. Contractor/Program Reviews

A total of 8 program reviews were held during this contract year.

1. The first program review was in the area of **Polymer Composites** and was held in Anaheim, California on 9 May 1997 at the Hilton Hotel. There were 9 presenters This was held in conjunction with the 42d SAMPE Symposium & Exhibition. UES provided travel for one advisor and honorarium for 4 advisors. UES provided acquisition of

meeting site including coffee breaks and continental breakfast and audio visual equipment. Dr. Charles Lee, Program Manager

2. The second program review was a joint ONR/AFOSR Nonlinear Optical Polymer review of research in the area of polymer science pertaining to optical applications. Two Multidisciplinary University Research Initiatives, an Accelerated Capabilities Initiative, and individual research efforts will be reviewed. The Air Force portion of the review was limited to second and third order NLO polymers and organics. Other topics such as photorefractive polymers were reviewed in a separate meeting. It was held 1-5 June 1997 at the Sea Turtle Inn, Jacksonville, Florida. Of the 43 attendees, 33 were speakers. ONR was the host; therefore, UES's role was to invite Air Force representatives and speakers.

Dr. Charles Lee, Program Manager

3. The third program review was entitled **High Energy Density Matter** (**HEDM**). It was held 1-3 June 1997 at the Westfields International Conference Center in Chantilly, Virginia. The HEDM Program is designed to search for new energetic forms of matter with possible future applications to Air Force propulsion and energy storage systems. Recent advances and accomplishments of the program and future program direction was outlined at this meeting. There were 62 in attendance of which 32 were speakers and 13 provided posters at the poster session. UES also provided on-site support, made all arrangements for the meeting including meals and audio visual equipment. UES provided travel and per diem for 3 advisors who attended the HEDM meeting.

Dr. Michael Berman, Program Manager

- 4. The fourth program review was in the area of **Tribology** and was held 24-26 June 1997 at the Holiday Inn in Englewood, Ohio. This was a joint Air Force/Navy meeting. Of the 54 in attendance, 36 were speakers. UES also provided on-site support, acquisition of meeting site and audio visual equipment.

 Major Hugh De Long, Program Manager
- 5. The **Chronobiology** program review was the fifth of the contract year. It was held 18-20 September 1997 at the Air Force Academy in Colorado Springs, Colorado. All funded research efforts in this program were reviewed. Invited Air Force laboratory scientists and relevant extramural scientists funded through the AFOSR Cognitive Sciences Program provided presentations. Of the 67 attendees, 31 gave oral presentations. UES provided travel and per diem for 10 advisors and honorarium for 7 advisors who attended the Chronobiology program review. UES also provided on-site support, made all arrangements for the meeting including meals and audio visual equipment.

Dr. Genevieve Haddad, Program Manager

6. The sixth program review was in the area of **Rocket Impact of Stratospheric** Ozone held at the National Academy of Sciences' Beckman Center in Irvine, California on

9 January 1998. The purpose of the meeting was to provide program progress and status of the work that has been carried out in the area of Atmospheric Effects of Rocket Exhausts. Twelve scientists assessed the progress and future direction of the program. UES provided acquisition of meeting site and audio visual equipment.

Dr. Michael Berman, Program Manager

7. The seventh program review was a joint Air Force/Navy review on **Electrochemistry**. It was held 15-16 January, 1998 in Ventura, California at the Doubletree Inn. The Air Force portion of the meeting focused on compact power. Of the 45 attendees, 38 were speakers. We provided travel expenses for one advisor. UES provided on site support, made all arrangements for the meeting including meals and audio visual equipment.

Major Hugh De Long, Program Manager

8. The final program review for this year was in the area of Nanoscale Devices and Novel Engineered Materials. It was held in Clearwater, Florida on 17-18 February 1998 at the Holiday Inn SunSpree Resort. UES provided on site support, made all arrangements for the meeting including meals and audio visual equipment. Eighteen people were in attendance.

Major Hugh De Long, Program Manager

C. Workshops

Two workshops were held during this year's effort.

- 1. The first workshop focused on **Composite Durability**. It was held at the Dearborn Inn in Dearborn, Michigan on 9 October 1997. Of the 17 in attendance, 11 provided talks. UES provided on site support, made all arrangements for the meeting including meals and audio visual equipment.
- Dr. Charles Lee, Program Manager
- 2. The second workshop was entitled **New World Vista Kickoff**, was held at the Marriott Riverwalk in San Antonio, Texas on 16 May 1997. Seventeen people were in attendance of which 11 provided talks. Some areas discussed were: Distributed Team Decision-Making and Performance in Complex Environments; Uninhabited Combat Air Vehicle (UCAV) Training Research Testbed; EEG-Based Online Cognitive Load Monitor; Integrated Cognitive, Computational and Biological Assessment of Workload in Decision Making. UES made all arrangements for the meeting including meals and audio visual equipment.

Dr. John Tangney, Program Manager

D. Panel Meetings

Four panel meetings were held during this year's effort.

1. A panel meeting was held on 20 May 1997 on **Durable Coatings** at WPAFB, Ohio. There were 9 presenters.

Dr. Charles Lee, Program Manager

2. A panel meeting was held on Molecular Dynamics and Theoretical Chemistry at the Hyatt Regency O'Hare Hotel, Rosemont, Illinois on 22 May 1997. Seven advisors reviewed proposals in the mentioned area. UES made arrangements for the meeting location. UES also provided travel, per diem and honorarium to the advisors. Reviews were secured from eighteen outside reviewers.

Dr. Michael Berman, Program Manager

3. A second Molecular Dynamics and Theoretical Chemistry panel meeting was held at the Hyatt Regency O'Hare Hotel, Rosemont, Illinois on 6 November 1997. Seven advisors reviewed proposals in the mentioned area. UES made arrangements for the meeting location. UES also provided travel, per diem and honorarium to the advisors. Reviews were secured from seventeen outside reviewers.

Dr. Michael Berman, Program Manager

4. The third panel meeting was on the subject of STTR and was held at the Holiday Inn Fairborn in Fairborn, Ohio on 3 February 1998. UES made arrangements for the meeting location. There were nine presentations along with Government meetings. Dr. Charles Lee, Program Manager

E. Advisors

In addition to advisors provided for Program Reviews, Workshops and Panel Meetings, UES provided travel, per diem and in many cases, honorarium for the following advisors:

Steven Zucker, Human Visual Processing, Air Force Office of Scientific Research, Bolling AFB, D.C.; 24 April 1997.

Tom Triscari, **Team Performance Measurement**, Air Force Armstrong Laboratory, Brooks AFB, Texas, 11-12 March 1997.

V. C. Ramesh, **Team Performance Measurement**, Air Force Armstrong Laboratory, Brooks AFB, Texas, 24-25 March 1997.

Martin Zatz, TARA Meeting, Arlington, Virginia, 17-20 March 1997.

Stephen Boppart, **Predictive Toxicology Initiative** and present a seminar on the use of optical coherence tomography in assessing potential teratogenic effects of toxic agents, Wright-Patterson Air Force Base, Ohio, 3 June 1997.

A. V. Phelps, Weakly Ionized Gases, USAF Academy, Colorado Springs, Colorado, 9-13 June 1997.

Lt Col David Brown, PRET Meeting, San Francisco Hilton, San Francisco, California, 11 June 1997.

Charles Woods, **Photorefractive Meeting**, University of California, San Diego, California, 26 July 1997.

Joan Fuller, 5th International Conference on Molten Salts, Dresden, Germany, 23-29 August 1997.

SUMMARY

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Judith M. Flory, Program Administrative Manager, and Donna Tinley, Assistant Program Administrator. Upon their retirements, Dr. Julien M. Christensen was replaced by Dr. Thomas Eggemeier as Program Manager and Betty Kerans was replaced by Ann Corbitt as Program Assistant. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

LIST OF APPENDICES

Breakdown of Research Proposals by Program Manager

Program for Polymer Composites Program Review, Hilton Hotel, Anaheim, California, 8 May 1997

Program for Nonlinear Optical Polymer Program Review, Sea Turtle Inn, Jacksonville, Florida, 1-5 June 1997

Program for **High Energy Density Matter (HEDM) Program Review**, Westfields International Conference Center, Chantilly, Virginia, 1-3 June 1997

Program for **Tribology Program Review**, Holiday Inn, Englewood, Ohio, 24-26 June 1997

Program for Chronobiology Program Review, Air Force Academy, Colorado Springs, Colorado, 18-20 September 1997

Program for Electrochemistry Program Review, Doubletree Inn, Ventura, California, 15-16 January 1998

Program for Nanoscale Devices and Novel Engineered Materials, Holiday Inn SunSpree Resort, Clearwater, Florida, 17-18 February 1998

Program for Composite Durability Workshop, Dearborn Inn, Dearborn, Michigan, 9 October 1997

Program for New World Vista Kickoff Workshop, Marriott Riverwalk, San Antonio, Texas, 16 May 1997

Program for Durable Coatings, WPAFB, Ohio, 20 May 1997

Program for Molecular Dynamics and Theoretical Chemistry, Hyatt Regency O'Hare Hotel, Rosemont, Illinois, 22 May 1997

Program for Molecular Dynamics and Theoretical Chemistry, Hyatt Regency O'Hare Hotel, Rosemont, Illinois, 6 November 1997

Program for STTR, Holiday Inn, Fairborn, Ohio, 3 February 1998

BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER

PROGRAM MANAGER	NO. OF PROPOSALS
Haddad	12
Tangney	18
Lee	15
Kozumbo	35
Bellaire	14
De Long	11
Berman	29
Roach	4

42nd International SAMPE Symposium and Exhibition

Anaheim Convention Center Anaheim, CA

"Basic Research Challenges in Polymeric Composite Materials and Processing." May 8, 1997, Room B2, Hall B

1:00-1:10	Opening Remarks Dr. Charles Lee, AFOSRNL
1:10-1:40	Air Force Basic Research Challenges for Structural Polymers and Polymeric Matrix Composites Dr. Charles Browning, WL MLB
1:40-2:10	High Temperture Composite Systems Dr. John Hoggatt, Boeing Company
2:10-2:40	Advanced Materials and Structures - Requirements for Future Research Mr. ('ecil Schneider, Lockheed-Martin
2:40-3:00	Break
3:00-3:30	High Performance Polymers and Composites: Basic Issues Dr. Norm Johnston, NASA Langley
3:30-4:00	Northrop Grumman's Prospective on Technology Voids in Polymer Composites M & P Mr. Robert Koon, Northrop Grumman
4:00-4:30	M & P Issues/Needs for PMCs at GE Aircraft Engines Dr. William McCormack, GE-Evansdale

SCHEDULE FOR 1997 ONR/AFOSR POLYMER PROGRAM REVIEW

Polymers for Electro-Optic Applications

Kenneth J. Wynne, ONR Program Manager Charles Y-C. Lee, AFOSR Program Manager

Sunday, 1 June

11:30 am	REGISTRATION
12:30 pm	Introductory Remarks - K. J. Wynne and C. Lee
1:00	Univ of AZIMURI Overview - Peyghambarian
1:45	Grubbs
2:15	Marks
2:45	BREAK
3:00	Jen
3:30	Marder
4:00	Kippelin
4:30	Perry
5:00	BREAK
5:15	Dirk
5:30	Rather
5:45	ADJOURN
6:00	Navy Panel - Wynne, et.al.

Monday, 2	June	Tuesday,	3 June
7:30 am 8:00	REGISTRATION & BREAKFAST Univ of MA MURI Review - Tripathy/Rubner	7:00 am 8:00	BREAKFAST Hammond
10:30	BREAK	8:30	Natansohn
10:45	USC ACI Review - Steier	9:00	Green
12:15 pm	LUNCH	9:30	Jenekhe
•		10:00	BREAK
		10:15	Stupp
		10:45	Tour
ONR-Funde	ed Individual Project Reviews	11:15	Asher
		11:45	LUNCH
		1:00 pm	Yu
1:30	Novak	1:30	Therein
2:00	Wright	2:00	Shashidhar
2:30	MacDiarmid	2:30	Heeger
3:00	BREAK	3:00	BREAK
3:15	Bazan	3:15	Lindsay
3:45	Epstein	3:45	Herman
4:15	ADJOURN	4:15	ADJOURN
4:30	Navy Panel	4:30	Navy Panel

Wednesday AFOSR-Fur	r, 4 June nded Individual Project Reviews	Thursday,	5 June
7:00 am 8:00 8:30 9:00 9:30 10:00 10:15 10:45 11:15	REGISTRATION & BREAKFAST Hopkins Pather Marder Dalton BREAK Heeger Prasad Forrest LUNCH	7:00 am 8:00 8:30 9:00 9:30 10:00 10:15 10:45 11:15	BREAKFAST Dudis Reinhardt Stegeman Spangler BREAK Jen Kenney Steier LUNCH
1:00 pm 1:30 2:00 2:30 3:00 3:15 3:45 4:15 4:15	Garito Thakur Peyghambarian Marks BREAK Caracci Ermer Kuzyk Dirk ADUCURN	1:00 pm 1:30 2:00 2:30 3:00 3:15 3:45 4:15 4:45 5:15	Perry Bjorkland Shi Chen BREAK Bischel Mustavich Tang Burzynski CLOSE

1997 High Energy Density Matter Contractor's Meeting Westfields International Conference Center Chantilly, VA 1-3 June 1997

Sunday, 1 June 1997

12:00 - 1:00	Registration ·
1:00 - 1:30	Introductory Remarks: Dr. Michael R. Berman, AFOSR
1:30 - 2:00	Propellant R&D for the Integrated High Pay-Off Rocket Propulsion Technology (IHPRPT) Program Dr. Patrick G. Carrick, Phillips Laboratory
2:00 - 2:30	Solid Rocket Propellants Present and Future Dr. Lou Cannuzzo, Thiokol Corporation
2:30 - 3:00	New Energetic Ingredients for High Performance Solid Propellants Dr. Kenneth O. Hartman, Alliant Techsystems
3:00 - 3:30	Break
3:00 - 3:30 3:30 - 4:00	Aspects of Solid and Liquid Propellant Development at Phillips Laboratory Dr. Tom W. Hawkins, Phillips Laboratory
	Aspects of Solid and Liquid Propellant Development at Phillips Laboratory
3:30 - 4:00	Aspects of Solid and Liquid Propellant Development at Phillips Laboratory Dr. Tom W. Hawkins, Phillips Laboratory Progress Towards Synthesis of Pentaprismane and Bicyclopropylidene: Potential Rocket Fuel Additives

Monday, 2 June 1997

8:30 - 9:00	New Methods for Excited States Dr. Rodney J. Bartlett, University of Florida
9:00 - 9:30	Theory and Synthesis of New High Energy Density Materials Dr. Karl O. Christe, Hughes STX Corporation
9:30 - 10:00	Synthesis of High-Energy Density Materials Based on Strained-Ring Compounds Dr. William P. Dailey, University of Pennsylvania
10:00 - 10:30	Break
10:30 - 11:00	Epoxidation Transition States and Stereoselectivity Modeling Dr. Kendall N. Houk, University of California, Los Angeles
11:00 - 11:30	Nitrogen Peroxides for HEDM Applications Dr. D. Scott Bohle, University of Wyoming
11:30 - 12:00	Models and Simulations of Energetic Materials Dr. Donald L. Thompson, Oklahoma State University
12:00 - 1:30	Lunch
1:30 - 2:00	The Role of Quantum Chemistry in the Design of High Energy Species Dr. Mark S. Gordon, Iowa State University
2:00 - 2:30	Reaction Field Cavity Optimization: A New Solvent Model for Electronic Structure Theory Dr. Teresa Head-Gordon, University of California, Berkeley
2:30 - 2:45	Direct Detection and Spectroscopy of O ₄ Dr. Holly Bevsek, University of California, Berkeley
2:45 - 3:15	Break

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Monday, 2 June 1997 (Cont'd)	

3:15 - 3:45	Computational Studies of High Energy Density Matter Dr. Gregory A. Voth, University of Utah
3:45 - 4:15	Spectral Theory of Physical and Chemical Binding: Aspects of Computational Implementation Dr. Peter W. Langhoff, Indiana University
4:15 - 4:45	Reactions of Laser-Ablated Boron Atoms with HCN. Infrared Spectra of BNC, BCN, HBNC and HBCN in Solid Argon. Reactions of Laser Ablated Aluminum Atoms with Ammonia. Infrared Spectra of HAINH ₂ , AINH ₂ and HAINH in Solid Argon Dr. Lester Andrews, University of Virginia
TBD	Workshop - Theory/Synthesis Discussion Leader: Dr. Jeffrey A. Sheehy, Phillips Laboratory
Tuesday, 3 June 199	77
8:30 - 9:00	Progress Towards the Production of Cryosolid HEDM Samples by Laser Ablation and Matrix Isolation Techniques Dr. Mario Fajardo, Phillips Laboratory
9:00 - 9:30	Characterization of Cryogenic Carbon and Boron HEDM Dr. C. William Larson, Phillips Laboratory
9:30 - 10:00	Theoretical Investigations of HEDM Dr. Jeffrey A. Sheehy, Phillips Laboratory
10:00 - 10:30	Break
10:30 - 11:00	Spectroscopy & Dynamics in Quantum Hosts Dr. V. Ara Apkarıan, University of California, Irvine
11:00 - 11:30	Mass Spectrometry of Doped Helium Clusters Dr. Kenneth C. Janda. University of California, Irvine
11:30 - 12:00	Light Metal Atom Interations with Hydrogen and Helium Clusters: Solvation Dynamics and Non-Adiabatic Effects Dr. Kevin Lehmann, Princeton University
12:00 - 1:30	Lunch

Tuesday, 3 June 1997 (Cont'd)

1:30 - 2:00	Spectroscopic Characterization of Non-Bonding Interactions of the Boron Atom Dr. Paul J. Dagdigian, Johns Hopkins University
2:00 - 2:30	Structure and Energetics of B(Ar) _n , B(N ₂), and O(H ₂) Clusters Dr. Millard H. Alexander, University of Maryland
2:30 - 3:00	Fundamental Insights from HEDM Studies Dr. David R. Yarkony, Johns Hopkins University
3:00 - 3:30	Break
3:30 - 4:00	Calorimetric Measurementds of O Atom Recombination Dr. Peter Taborek and Dr. James E. Rutledge, University of California, Irvine
4:00 - 4:30	Characterization of Metal Atom-Doped Cryogenic Solids Dr. George M. Seidel, Brown University
4:30 - 5:00	Ozone in Solid Oxygen Dr. Richard A. Copeland, SRI Interational
5:00 - 5:30	Advanced Cryogenic Solid Hybrid Rocket Engine Developments for HEDM and Non-HEDM Demonstrations Mr. Eric E. Rice. Orbital Technologies Corporation (ORBITEC)

Tribology Program Review Holiday Inn, Englewood, Ohio 24-26 June 1997

Tuesday, 24 June 1997

0840	Introduction Major Hugh Delong, AFOSR, and Dr. Peter Schmidt, ONR
0900	Soft and Hard Junctions. Dr. Uzi Landman, Georgia Institute of Technology
0930	Kelvin Probe Measurements for Wear Monitoring, Dr. Steve Danyluk, Georgia Institute of Technology
1000	Tribological Behavior of Polycrystalline Diamond and Poly-/Single-Crystal Silicon in Vacuum and Hydrogen for MEMS Micromechanism Applications, Dr. Michael N. Gardos, Hughes Aircraft Company
1030	Break
1045	Fluorination of Diamond Surfaces by Irradiation of Adsorbed Perflorinated Alkyl Iodides, Dr. John T. Yates, Jr., University of Pittsburgh
1115	Nanotribological Studies of Bulk Ceramic Materials, Multilayered Thin Films, and Liquid Lubricant Films, Dr. Bharat Bhushan, Ohio State University
1145	Force Microscopy Studies of Tribology at the Nanometer Scale: Probing the Molecular Origins of Friction, Dr. Charles M. Lieber, Harvard University
1215	Lunch
1400	Tribology in Extreme Environments, Dr. Jeff S. Zabinski, WL/MLBT
1430	Advanced Carbon Based Coatings for Wear and Friction Reduction, Dr. Andrey A. Voevodin, WL MLBT
1500	Lubricious Oxides, Dr. Somuri V. Prasad, WL/MLBT
1530	Break

1545	The Surface Chemistry and Tribology of Carbide and Nitride Hard Coatings, Dr. Scott S. Perry, University of Houston
1615	The Application of Raman Microscopy to the Friction, Wear and Tribochemistry of Solid Lubricating Films, Dr. Larry E. Seitzman, Naval Research Laboratory
1645	Tribological Studies Using the Surface Forces Apparatus (SFA) and the X-SFA. Dr. Jacob Israelachvili, University of California, Santa Barbara
1715	Electrostatic Charging Precursor to Scuffing in Lubricated Contacts. Dr. Robert J. K. Wood, University of Southhampton
Wednesday,	25 June 1997
0830	Recent Progress Towards First-Principles Predictions of Fracture Strengths and Wear Resistance of Polycrystalline Covalent Ceramics, Dr. Donald W. Brenner, North Carolina State University
0900	Diffusion Mechanisms of Vapor Phase Lubricants, Dr. Nelson H. Forster, WL POLS
0930	Integrated Diagnostics, Dr. Richard S. Cowan, Georgia Institute of Technology
1000	Break
1015	Surface Treatments for Probing of Tribological State Variables, Dr. Ursula Gibson, Dartmouth College
1045	Temperature Probes for Detecting Incipient Failure of Tribological Components, Dr. Francis E. Kennedy, Dartmouth College
1115	A Thermal-Tribological Approach for Designing Tribological Elements and Its Applications to Engine Pistons and Journal Bearings, Dr. Qian (Jane) Wang, Florida International University
1145	New Spectroscopic and Theoretical Probes of Tribochemical Processes, Dr. Dor Ben-Amotz, Purdue University
1215	Lunch

1400	The Nature of Tribochemistry and the Effectiveness of BL Films, Dr. Stephen M. Hsu, University of Maryland	
1430	Deformation Behavior of Thin Liquid Films at Elevated Pressure, Dr. Scott Bair, Georgia Institute of Technology	
1500	High-Temperature Liquid Lubricant and Additive Research, Dr. Harvey L. Paige, WL MLBT	
1530	Break	
1545	Fundamental Studies of the Interactions of Perfluoropolyalkylether Based Fluids with Iron Containing Surfaces, Dr. Jeffrey Sanders, WL/MLBT	
1615	Nanorheology in the Service of Tribology with Emphasis on Perfluoroethers. Dr. Steve Granick, University of Illinois	
1645	Tribological Properties of Molecular Monolayers on Metal Surfaces, Dr. Andrew J. Gellman, Carnegie Mellon University	
1715	Materials Degradation and Fatigue Under Extreme Conditions, Dr. Jiri Jonas, University of Illinois	
Thursday, 26 June 1997		
0830	Nanoarches and Nucleation and Growth of Cubic Boron Nitride, Dr. Laurence D. Marks, Northwestern University	
0900	Molecular Dynamics Investigations of the Tribology of Hydrocarbons, Dr. Judith A. Harrison, US Naval Academy	
0930	Molecular Dynamics Simulations of Ceramics, Dr. John W. Mintmire, Naval Research Laboratory	
1000	Break	
1015	Variational Fitting and Quantum-Chemical Nanotribology, Dr. Brett I. Dunlap, Naval Research Laboratory	
1045	Theory of Scanning Tunneling Microscopy (STM) Spectra Through Molecular Adsorbates: Investigating Charge Structure and Charge Flow at a Molecule Functionalized Metal Surface, Dr. Mark Ratner,	

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1115	Determining the Interactions Between Polymer-Coated Surfaces Through Theory and Simulation, Dr. Anna C. Balazs, University of Pittsburgh
1145	Lattice and Continuum Models of Some Mechanical Properties of S-P Metals and Directionally Bonded Semiconductors, Dr.: Norman H. March, Oxford University
1215	Adjourn

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Chronobiology and Neural Adaptation Program Review United States Air Force Academy Colorado Springs, Colorado 18-20 September 1997

Thursday, 18 September 1997

0730	Registration/Continental Breakfast
0830	Introduction Dr. Genevieve Haddad, AFOSR
0900	Organization of the Human Circadian System Dr. Robert Y. Moore. University of Pittsburgh
0930	PRET95 Homeostatic and Circadian Regulation of Wakefulness During Jet Lag and Sleep Deprivation: Effect of Wake-Promoting Countermeasures on the Development of Neurobehavioral Deficits Dr. David F. Dinges. University of Pennsylvania School of Medicine
1000	The Effect of Caffeine on the Circadian and Homeostatic Interaction Underlying the Deterioration of Neurobehavioral Functioning During Jet Lag and Sleep Deprivation Dr. Derk-Jan Dijk. Brigham & Women's Hospital, Harvard Medical School
1030	Break
1100	The Effect of Exercise on Endogenous Circadian Period. Sleep and Performance Dr. Charles A. Czeisler, Brigham & Women's Hospital, Harvard Medical School
1130	Circadian Phase Alters the Cost of Paying Attention Dr. Jeremy Wolfe, Brigham & Women's Hospital, Harvard Medical School
1200	Break
1215	Effects of Light, Exercise and Manipulations of the Sleep-Wake Cycle on Human Circadian Rhythms Dr. Eve Van Cauter, University of Chicago

1245	Circadian and Metabolic Modulation of Human Vision Dr. Robert B. Barlow, SUNY Health Science Center
1315	Lunch
1430	Air Force Basic Research Program on Human Chronobiology and Sleep Dr. Rod J. Hughes. Air Force Research Laboratory, Brooks AFB
1500	Crew Fatigue During Simulated, Long Duration B-1B Bomber Missions Dr. Jonathan French, Air Force Research Laboratory, Brooks AFB
1530	Verbal Communication in Team Situational Awareness Dr. Linda R. Elliott, Air Force Research Laboratory, Brooks AFB
1600	Break
1615	Learning Abilities Measurement Program. Individual Differences Dr. Pat Kyllonen, Air Force Research Laboratory, Brooks AFB
1645	Individual Differences in Diurnal Preference Dr. Richard D. Roberts, Air Force Research Laboratory, Brooks AFB
1715	EEG Pattern Recognition of Individual Differences in Cognitive Abilities Dr. Alan Gevins, SAM Technology
1900	Dinner at Officers Club
1945	Air Force Operational Viewpoint, Speaker, Col Dale Hammer, United States Air Force Academy, Colorado Springs
Friday, 19 S	eptember 1997
0830	Continental Breakfast
0900	Control of Circadian Behavior by Transplanted Suprachiasmatic Nuclei Dr. Michael Menaker, University of Virginia
0930	Dissecting the Mammalian SCN Dr. Rae Silver, Columbia University
1000	Break
1015	Neural Stem Cells - Transplantation and the Circadian System Dr. William J. Schwartz, University of Massachusetts Medical School

1045	Organization Within and Among Vertebrate Circadian Oscillators Dr. Gene D. Block, University of Virginia	
1115	Break	
1130	Cellular Analysis of Circadian Rhythmicity in Cultured SCN Neurons Dr. Steven M. Reppert, Massachusetts General Hospital	
1200	Intracellular Electrophysiology of the Rat Suprachiasmatic Nucleus: Membrane Properties. Neurotransmission and Effects of Neuromodulators Dr. F. Edward Dudek. Colorado State University	
1230	Lunch	
1400	Modulation of Neuronal Activity in the Suprachiasmatic Nucleus Dr. Anthony N. van den Pol, Yale University Medical School	
1430	Synaptic Plasticity and Memory Formation Modifying the Operation of AMPA-Type Glutamate Receptors: Memory Encoding and a Novel Pharmoacology Dr. Gary Lynch, University of California, Irvine	
1500	Break	
1515	Dynamic Reconfiguration of a Pattern Generating Neural Network Dr. John H. Byrne. University of Texas-Houston Health Science Center	
1545	Gene Regulation in Memory Formation and Circadian Rhythm Dr. Arnold Eskin. University of Houston	
1700	Macaroni Grill	
Saturday, 20 September 1997		
0830	Continental Breakfast	
0900	Neurophysiological and Behavioral Analysis of Circadian Rhythm Entrainment Dr. Benjamın Rusak, Dalhousie University	
0930	Neural Regulation of Non-Photic Entrainment	
	Dr. Lawrence P. Morin, Stony Brook University	

1015	Neurochemical Regulation of Circadian Phase Dr. Michael A. Rea, Air Force Research Laboratory, Brooks AFB
1045	Different Areas of the Brain May be Involved in Fear vs. Anxiety Dr. Michael Davis, Yale University
1115	PRET95 Homeostatic and Circadian Regulation of Wakefulness During Jet Lag and Sleep Deprivation: Effect of Wake-Promoting Countermeasures. Pre-Clinical Assessment of Compensatory Sleep Responses to Drug-Induced Waking Dr. Dale M. Edgar, Stanford University
1145	Lunch
1300	Interaction of Light and Clock Regulation in Neurospora Dr. Jennifer J. Loros. Dartmouth Medical School
1330	Probing the Drosophila Circadian System Using Enhancer Detectors Dr. Paul E. Hardin, University of Houston
1400	Break
1430	Circadian Rhythms in Zebrafish and Genetic Analysis of Vertebrate Circadian Rhythmicity Dr. Gregory M. Cahill. University of Houston
1500	Genetic Analysis of Daily Activity in Humans and Mice Dr. Joseph S. Takahashi. Northwestern University
1530	Closing Remarks
1800	Chuckwagon Sugger at Flying W Ranch

AFOSR/ONR Electrochemistry Science & Technology Review

Doubletree Hotel, Ventura, California 15-16 January 1998

Thursday, 15 January 1998

0700	Registration/Continental Breakfast
0800	Introduction Dr. Richard T. Carlin, ONR, and Dr. Hugh C. De Long, AFOSR
0815	Nanocomposite Polymer Electrolytes. Dr. Emmanuel P. Giannelis, Cornell University
0840	Properties of Fuel Cell and Battery Materials. Dr. P. E. Stallworth, Dr. John J. Fontanella, Dr. M. C. Wintersgill, Dr. C. A. Edmondson, U. S. Naval Academy
0905	NMR Investigations of Materials for Batteries & Fuel Cells, Dr. Steve Greenbaum. Hunter College of CUNY
0930	Polymeric Gels as an Environment for Electrochemistry, Dr. Malgorzata Ciszkowska, Brooklyn College
0950	Low Dimensional Fast Ion Conductors. Dr. Larry G. Scanlon, Air Force Research Laboratory
1015	Break
1030	Single Lithium Ion Conducting Polymer Electrolyte, Dr. William A. Feld, Wright State University
1055	Synthesis of a Mesomorphic, Columnar Porphyrin for Fast Li Ion Conducting Electrolytes. <i>Dr. John Arnold</i> , <i>University of California</i> , <i>Berkeley</i>
1120	X-Ray Absorption Structural and Electrochemical Studies of Novel Materials for Advanced Batteries and Ultracapacitors, Dr. Azzam N. Mansour, Naval Surface Warfare Center

1140	Remediation of Aqueous Waste by Electrified Microheterogeneous Catalysis. Dr. Debra Rolison, Naval Research Laboratory
1205	Lunch
1330	Electrochemical Properties of Sol-Gel Derived Materials, Dr. Bruce Dunn. University of California, Los Angeles
1355	Electroanalytical Investigations of Sol-Gel Derived Materials, Dr. Maryanne M. Collinson, Kansas State University
1420	Development of New Trace Analytical Capabilities at the Electrode/Solution Interface and Their Application to a Novel Thin Film Battery System. Dr. Daniel A. Buttry, University of Wyoming
1445	Clay-Templated Nanoporous Graphitic Carbon Electrodes for Secondary Batteries. Dr. Mahmoud Aldissi. Dr. E. Lazaro, Dr. M. Bhamidipati and Dr. B. Dixon, Cape Cod Research
1510	Break
1525	Nanofibrils Carbon Electrode for Rechargeable Batteries, Dr. Chuanjing Xu., Nanomaterials Research Corporation
1550	Composite Nanoscale Cathodes for Li-Ion Batteries, Dr. Michael C. Kimble, Physical Sciences, Inc.
1615	Electrocatalysts Based on Electrode-Confined Dendrimers, Dr. Richard M. Crooks, Texas A&M University
1640	The Solution Phase Catholyte Semi Fuel Cell Utilizing a Flowing Aqueous Electrolyte, Dr. Eric G. Dow and Dr. Maria G. Medeiros, Naval Undersea Warfare Center
1700	Electrode Surface Modification for Cathode Catalysis in Semi-Fuel Cells, Dr. Russell R. Bessette and Dr. James M. Cichon, University of Massachusetts, Dartmouth
1725	Break
1800	Semi-Fuel Cell Mini-Symposium

Friday, 16 January 1998

0745	Continental Breakfast
0825	Probing Step Density Effects on Reactions at Single Crystal Electrodes, Dr. Carol Korzeniewski, Texas Tech University
0850	Electrodeposition Dynamics and Redox Probe Microscopy, Dr. Hector D. Abruna. Cornell University
0915	Phase Dynamics and Rate/Structure Correlations in Electrocatalytic Nanoclusters. Dr. Ralph G. Nuzzo, Dr. John R. Shapley, Dr. Anatoly I. Frenkel, Dr. Michael S. Nashner, and Dr. Charles W. Hills, University of Illinois, Urbana-Champaign
0940	Metallic Monolayers as Fuel Cell Electrode Catalysts, Dr. Stanley D. James, Naval Surface Warfare Center
1000	Break
1015	New Opportunities in Fundamental Nanoelectrochemistry and Bioelectrochemistry, Dr. Charles R. Martin, Colorado State University
1040	Studies of Latent Acidity and Neutral Buffered Chloroaluminate Ionic Liquids, Dr. Robert A. Osteryoung, North Carolina State University
1105	Developing Lithium Thermal Batteries for Navy and Joint-Service Air- Launched Weapons, Dr. Carl H. Hinners, Naval Air Warfare Center
1125	Applications of Ambient-Temperature Ionic Liquids to Compact Power Sources and Electrodeposition of Advanced Aluminum Alloys, <i>Dr. Paul C. Trulove</i> , <i>U. S. Naval Academy</i>
1150	Double Layer Studies at Single-Crystal Electrodes in Non-Aqueous Solutions, Dr. W. Ronald Fawcett, University of California, Davis
1215	Lunch
1330	Two Facets of Electron Transfer: Solvent Dynamics and Charge Transfer, Electron-Molecule Collision Insight into Organic Halide Anion Potential Energy, Dr. Rudolph A. Marcus. California Institute of Technology
1355	Electron Transfer at Nanoscale Electrochemical Interfaces, Dr. Joseph T. Hupp, Northwestern University

1420	Charge Transfer Systems of Molecular Dimensions, <i>Dr. Royce W. Murray</i> , <i>University of North Carolina</i>
1445	The Response of Water in High Surface Electric Fields. Dr. Eric M. Stuve, University of Washington
1510	Electric Fields, Dr. Henry S. White, University of Utah
1535	Break
1550	Electrochemical Growth of Heteroepitaxial Layers of Low-Dimensional Conductors, Dr. Daniel E. Hooks and Dr. Michael D. Ward, University of Minnesota
1615	Catecholamine Secretion from Single Cells. Dr. R. Mark Wightman, University of North Carolina at Chapel Hill
1640	Understanding the Mechanism of Ennoblement of Stainless Steels, Dr. Zbigniew Lewandowski, Montana State University
1705	A Hybrid Electrochemical/Chemical Method for the Epitaxial Synthesis of Compound Semiconductor Nanocrystallites on Graphite, Dr. Reginald M. Penner, University of California, Irvine
1730	Electrochemical Assembly of Nanophase Metal Oxides. Dr. Jay A. Switzer, University of Missouri, Rolla
1755	Polymerized Phthalocyanines for Electrochemical Applications, Dr. Peter W. Faguy, University of Louisville
1820	Closing Remarks

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AGENDA

2nd Annual Review of AFOSR MURI "Nanoscale Devices and Novel Engineered Materials" University of Florida

Monitor:

Maj. H.C. DeLong, Ph.D.

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February 17, 1998

Location:

Coral Room A, Holiday Inn Sun Spree Resort

Clearwater Beach, Florida

9:00 am Welcome and Overview of Program -- S.J. Pearton (MSE/UF)
9:15 am Program Goais and Achievements -- J.R. Childress (MSE/UF)

Novel Engineered Materials and Properties

9:30 am	Nanoparticle Dispersions in Polymer Matrices E.P. Goldberg (MSE/UF)
10:00 am	COFFEE BRLAK
10:30 am	Porous Si R.E. Hummel (MSE/UF)
11:20 am	Molecular Cluster Calculations on Display Materials J Lewis (MSE/UF)
11:35 am	Pulsed Laser Deposition of Nanoparticle Y ₂ O ₂ :Eu S. Jones (MSE/UF)
12:00 Noon	LUNCH
1:30 pm	Mechanical Properties of Nanostructured Materials S.A. Syed Asif (NRL)

Advanced Nanostructures

2:00 pm	Quantum Effects in Magnetic and Superconducting Materials I.K. Schuller
	(Physics/UCSD)
2:45 pm	COFFEE BREAK
3:15 pm	Integration of Magnetic Nanoparticles with 2D Electron Systems S. von Moinar
	(Physics/FSU)
4-5:30 pm	Discussion (all)

Wednesday

February 18, 1998

Location:

Coral Room A

Submicron Magnetic Structures: Theory, Deposition and Processing

9:00 am	Overview J.R. Childress (MSE/UF)
9:15 am	Nanoscale Patterning F. Sharifi (Physics/UF)
10:00 am	Novel Magnetoresistive Materials J.R. Childress (MSE/UF)
10:45 am	COFFEE BREAK
11:15 am	Fabrication. Deposition and Characterization in Support of Magnetic Sensor
	Development D. Temple (MCNC)
12:00 Noon	LUNCH
1:30 pm	Theory & Modelling of GMR S. Hershfield (Physics/UF)
2:15 pm	Dry Etching of Magnetic Materials - S.J. Pearton (MSE/UF)
3:00 pm	COFFEE BREAK
2:30-4:00 pm	Summary/Future Plans – S.J. Pearton (MSE/UF)
4-5:30 pm	Discussion (all)

AFOSR COMPOSITE DURABILITY WORKSHOP

9 October 1997

Dearborn Inn, Dearborn, MI

730	Continental Breakfast
830	Charles Lee
845	Ozden Ochoa
900	Morgan
915	Yee
930	Leung
945	coffee break
1000	Seferis
1015	Curliss
1030	Reifsnider
	Piggott
	Kumosa
	Whitcomb
1130	Daniel
1145	Lunch
1300	Round Table Discussion
1400	break

1700 adjourn latest

AGENDA

Air Force New World Vistas 'People' Research

Air Ford	orce New World Vistas "People" Research				
Kick-off 16-May	off Meeting lay-97				
0830	CONVENE AT SALON B	, MARRIGTT RIVERWALK HOTEL, SAN ANTONIO TX			
0830	Dr. Brendan Godfrey	AF Armstrong Laboratory Welcome/Introduction			
0845	Or. John F Tangney	AF Office Scientific Research Program Overview			
0900	Or. Linda R Elliott	AF Armstrong Lab Distributed Team Decision-Making and Performance in Complex Environments			
0915	Dr. Elizaceth Martin	AF Armstrong Laboratory Uninnabited Combat Air Vehicle (UCAV) Training Research Testoed			
0930	Or. Eilen ⊢all	AF Armstrong Laboratory Cognitive Engineering for Team Tasks			
0945	Or. Alan S. Gevins	SAM Technology EEG-Based Online Cognitive Load Monitor			
1000	BREAK				
1020	Dr. Michael W. Haas	AF Armstrong Laboratory Understanding Attentional Mechanisms Underlying Increases in Performance Associated with Multi-Dimensional Displays			
1035	Dr. Robert H. G.lkey	Wright State University Cognitive Workload in a Complex Synthetic Task Environment: The Role of Functional Display and Control Representations			
1050	Or. Phillip L. Ackerman	University of Minnesota Cognitive Modeling and Task Analysis			
1105	Or. F. Javier Lerch	Carnegie Mellon University Integrated Cognitive, Computational and Biological Assessment of Workload in Decision Making			

AF Armstrong Laboratory
Training Research for Automated Instruction (TRAIN)

1135 ADJOURN 13-May-97

Dr. Wes Regian

1120

AFOSR DURABLE COATINGS PANEL REVIEW

Room 354, Polymer Branch Building 654 Wright-Patterson AFB, OH

20 May 1997

0830	Closed Meeting Government and Advisors Only
0900	Opening Remarks Charles Y-C Lee, AFOSR
0915	ML Coating Effort Arnold Donley, Wright-Patterson AFB
0945	ML 6.1 Effort Fred Arnold, Wright-Patterson AFB
1015	Break
1030	Dharmaraj Raghavan Howard University
1100	Mark Soucek North Dakota State University
1130	Yanching Jean University of Missouri - Kansas
1200	Lunch
1300	J. R.Reynolds University of Florida
1330	Paras Prasad SUNY at Buffalo
1400	Thomas Serry University of Connecticut
1430	General Discussions/Adjournment

SUMMARY OF REVIEWS AFOSR Molecular Dynamics Panel Meeting

97-NL-102 Ion and Neutral Dynamics of Ceramic Materials Formation and Atmospheric Processes

- Stephen R. Leone, University of Colorado

Laurie J. Butler, University of Chicago (A-/2/3)
Steven D. Colson, Pacific Northwest National Laboratory (A+/2)
Charles S. Parmenter, Indiana University (A/A+/3)
James C. Weisshaar, University of Wisconsin (A/1)
J. Michael White, University of Texas at Austin (A/B+/3)

97-NL-137 The Growth of Nanostructures and Composite Films on Solids: Simulations and Phenomenological Theory

- Hona L. Metiu, University of California

Jeffrey Hay, Los Alamos National Laboratory (A/3)
Hannes Jonsson, University of Washington (A+/1)
Max G. Lagally, University of Wisconsin-Madison (A-/2)
J. Michael White, University of Texas at Austin (A+/3/4)

97-NL-152 Theoretical Studies of Group IVA and Group IVB Chemistry

- Mark S. Gordon, Iowa State University

Christopher J. Cramer, University of Minnesota (A+/1) Larry Harding, Argonne National Laboratory (A/3) Jeffrey Hay, Los Alamos National Laboratory (A/1) George Schatz, Northwestern University (A/1) Jack Simons, University of Utah (A-/1)

97-NL-153 Study of Complex Kinetic Systems with Imposed Variation of Temperature - John Ross, Stanford University

William L. Hase, Wayne State University (B/4)

Jeffrey Hay, Los Alamos National Laboratory (*/5)

Joel E. Keizer, University of California, Davis (B/B+/1)

Davis W. Oxtoby, University of Chicago (A/3)

George Schatz, Northwestern University (A/3)

*Note: Letter grade not given.

97-NL-156 Femtosecond Dynamics of Chemical Reactions

- Almed H. Zewail, California Institute of Technology

Laurie J. Butler, University of Chicago (A-/2)

Steven D. Colson, Pacific Northwest National Laboratory (A+/2)

Edward R. Grant, Purdue University (A+/3)

Charles S. Parmenter, Indiana University (A-/3)

James C. Weisshaar, University of Wisconsin (A/4)

97-NL-157 Microwave Cavity Spectroscopy

- Richard N. Zara, Stanford University

Laurie J. Butler, University of Chicago (A-/2/4)

Steven D. Colson, Pacific Northwest National Laboratory (A-/3)

Paul L. Houston, Cornell University (A-/3)

Charles S. Parmenter, Indiana University (A-/3/4)

James C. Weisshaar, University of Wisconsm (A/3)

97-NL-158 Dynamical Spectroscopy of Prototypes in Condensed Phase Chemistry

- V. Ara Apkanan, University of California

Laune J. Butler, University of Chicago (A/2/5)

Charles S. Parmenter, Indiana University (A/A-/4/5)

George Schatz, Northwestern University (A/2)

Norbert F. Scherer, University of Pennsylvania (A/A/1)

James C. Weisshaar, University of Wisconsin (B+/5)

97-NL-159 Energy Transfer Kinetics and Dynamics of Relevance to Iodine Lasers

- Michael C. Heaven, Emory University

Laurie J. Butler, University of Chicago (A-/B+/2)

Steven D. Colson, Pacific Northwest National Laboratory (B+/3)

John B. Koffend, Los Angeles (A-/1)

Charles S. Parmenter, Indiana University (B+/2)

James C. Weisshaar, University of Wisconsin (A-/3)

97-NL-160 Theoretical Studies of Gas Phase Elementary Reactions

- Keiji Morokuma, Emory University

Clifford E.Dykstra, Indiana University, Purdue (A-/2/3)

William L. Hase, Wayne State University (A/2)

Jeffrey Hay, Los Alamos National Laboratory (A/1)

George Schatz, Northwestern University (A-/1)

Jack Simons. University of Utah (A-/1)

97-NL-161 Electronic. Phonon and Optical Properties of the Polyhedral Cage Materials: Si and Ge Clathrates

- Peter C. Eklund, University of Kentucky

Sanford A. Asher, University of Pittsburgh (B+/4)

Steven D. Colson, Pacific Northwest National Laboratory (A/4)

Robert L. Whetten, Georgia Institute of Technology (A+/2)

J. Michael White, University of Texas at Austin (A-/4)

97-NL-166 Atomistic Simulations of High-Temperature Ceramics Metal/Ceramic Interfaces. and MEMS on Parallel Computers

- Rajiv K. Kalia, Louisiana State University

Donald E. Ellis, Northwestern University (A/1)

Jeffrey Hay, Los Alamos National Laboratory (A-/2)

John Mintmure, Naval Research Laboratory (A/1)

George Schatz, Northwestern University (A/3)

J. Michael White, University of Texas at Austin (A-/3/4)

97-NL-169 Fundamental Studies of Ions and Ionic Processes

- Henry F. Schaefer III, University of Georgia

Clifford E. Dykstra, Indiana University-Purdue (A/1/2)
Jeffrey Hay, Los Alamos National Laboratory (A-/1)
J. Vince Ortiz, Kansas State University (A/2)
George Schatz, Northwestern University (A-/A/1)

SUMMARY OF REVIEWS AFOSR Molecular Dynamics/Theoretical Chemistry Review Panel Meeting

97-NL-172 Intramolecular Vibrational Energy Transfer and Bond-Selected Photochemistry in Liquids

- F. Fleming Crim, University of Wisconsin

Laurie J. Butler, University of Chicago (A-/2)
Hai-Lung Dai, University of Pennsylvania (A-/3)
George W. Flynn, Columbia University (A/2)
Charles S. Parmenter, Indiana University (A/2)

97-NL-342 Linear Scaling Density Functional Theory With Periodic Boundary Conditions

- Gustavo E. Scuseria, Rice University

Michael Colvin, Lawrence Livermore Laboratories (A/2) Richard A. Friesner, Columbia University (A/1) Peter M.W. Gill, University of Cambridge, UK (B+/1) Jeffrey Hay, Los Alamos National Laboratory (A-/2) George C. Schatz, Northwestern University (A/2)

97-NL-346 Electronic Processes Governing Non-Adiabatic Photodissociations and Chemical Reactions

- Karl F. Freed, The University of Chicago

Ernest R. Davidson, Indiana University (A-/1)
Jeffrey Hay, Los Alamos National Laboratory (A./2)
Morris Krauss, CARB/NIST (A/1)
George C. Schatz, Northwestern University (A/2)
Donald G. Truhlar, University of Minnesota (A/1)

97-NL-356 Stability, Growth and Reactivity at High Temperature Intermetallic Surfaces

- Talat S. Rahman, Kansas State University

Charles T. Campbell, University of Washington (B+/3)
Steven D. Colson, Pacific Northwest National Laboratory (A-/4)
Bruce E. Koel, University of Southern California (B+/3)
J. Michael White, University of Texas at Austin (A/3)

97-NL-361 "Reactive" Vibrational Relaxation in the Gas-Phase and on Surfaces

- Alec M. Wodtke - University of California

Laurie J Butler, University of Chicago (A-/2)

Steven D. Colson, Pacific Northwest National Laboratory (A/3)

Paul L. Houston, Cornell University (A/1)

Charles S. Parmenter, Indiana University (A/2)

James C. Weisshaar, University of Wisconsin (A/2)

97-NL-362 Controlled Forward and Inverse Chemical Dynamics

- Herschel Rabitz, Princeton University

Paul W. Brumer, University of Toronto (A-/1)

David Hoffman, Iowa State (A/3)

Stuart A. Rice, University of Chicago (A/1)

George C. Schatz, Northwestern University (A/2)

97-NL-364 Simulation of Reaction Dynamics: Nonadiabatic and Solvation Effects

- Sharon Hammes-Schiffer, University of Notre Dame

Jeffrey Hay, Los Alamos National Laboratory (A/3)

Edward F. Haves. Ohio State University (B/2-3)

Anne B. McCov, Ohio State University (B+/4)

George C. Schatz, Northwestern University (A/1)

Donald G. Truhlar, University of Minnesota (A+/1)

James C. Weisshaar, University of Wisconsin (A/4)

J. Michael White, University of Texas at Austin (?/4)

97-NL-369 Dynamics of Molecule-Surface Interactions on Metal Oxides

- Curt Wittig, University of Southern California

Laurie J. Butler, University of Chicago (A/2/3)

Steven D. Colson, Pacific Northwest National Laboratory (A+/3)

Charles S. Parmenter, Indiana University (A-/4)

Charles T. Rettner, IBM Almaden Research Center (A/1)

James C. Weisshaar, University of Wisconsin (A/3)

J. Michael White, University of Texas at Austin (A+/1)

97-NL-417 Experiments in Molecular Optics

- Robert J. Gordon. University of Illinois. Chicago

Laurie J. Butler, University of Chicago (A+/A/A-/3)

Steven D. Colson, Pacific Northwest National Laboratory (A-/3)

Charles S. Parmenter, Indiana University (A/4)

George C. Schatz, Northwestern University (A/3)

James C. Weisshaar, University of Wisconsin (A/3)

STTR PROGRAM REVIEW

February 3, 1998
Meeting Room II
Holiday Inn Conference Center
Dayton, Ohio

8:30 - 8:45	Government Only Session
9:00	Open Session Begins
9:00 - 9:15	Comments by Charles Lee (Topic Manager) and Chris Hughes (STTR Manager at AFOSR)
9:15- 9:45	Sentel Technologies-EO Fiber
9:45-10:15	F&S-Ionic Self Assembly Monolayer
10:15-10:45	Break
10:45-11:15	PD-LD-Self Assembly Organical Chemical Beam Deposition
11:15-11:45	Pacific Wave Industries-New Directions in NLO Materials
11:45-12:15	Los Gatos Research-NLO Thin Film for Inspection
12:15-13:15	Lunch
13:15-13:45	Optivision-Development of In-line Fiber Devices
13:45-14:15	EIC Laboratories-Regioregular NLO Polymers
14:15-14:45	MetroLaser, IncNovel Organic Film for Real Time Holographic Signal Processing
14:45-15:15	Break
15:15	Closed Session Begins
15:15-15:45	Cornerstone-Glass Forming LC for Photonic Devices
15:45-16:45	Government Only Session

APPENDIX M

ANNUAL REPORT

CHEMISTRY AND LIFE SCIENCES RESEARCH PROGRAM CONTRACT NO. F49620-95-C-0026

Period of Performance: 3/1/98 - 2/28/99

Prepared For:

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH CHEMISTRY AND LIFE SCIENCES DIRECTORATE

Dr. Genevieve Haddad, Program Manager

Presented By:

UES, Inc. 4401 Dayton-Xenia Road Dayton, OH 45432-1894

INTRODUCTION

UES, Inc. is providing research evaluation services to the Directorate of Chemistry and Life Sciences, Air Force Office of Scientific Research (AFOSR), in subareas that include Neurosciences (e.g., Neurochemistry, Biology, Electrophysiology, Neuroanatomy, Multisensory Integration/Spatial Orientation, Cardiovascular Physiology, and Bioenvironmental Hazards; Psychophysics, Psychophysiology, Physiological Psychology, Sensation, Perception, Cognition); Computer Sciences (e.g., Vision and Robotics); Otolaryngology; Meteorology, Chemistry (e.g., computational chemistry, polymeric and organic materials, photonic materials, inorganic and surface chemistry, high density materials); Biotechnology (e.g., materials and processes); and Fuels (e.g., petroleum and synthetic); and in related programs under development.

The services provided by UES, Inc. include: selecting qualified scientists to evaluate proposals, assembling scientific groups to evaluate, analyze and advise on content and direction of Chemistry and Life Sciences Programs; organizing workshops to assist in the definition of new basic research areas proposed by the Chemistry and Life Sciences Directorate; providing advisors to make presentations and assist government personnel with analyzing areas of relevant science; and providing advisors to assist and advise on site visits to research laboratories.

The third option year included: 66 Proposals that were reviewed; 3 Program/Contractor Reviews; 3 Workshops and 1 Panel Meeting.

A. Evaluations of Individual Research Proposals

UES sent out 66 proposals to 196 evaluators during the performance period of 1 March 1998 through 28 February 1999.

UES has been providing the Directorate of Chemistry and Life Sciences a Summary of Proposals Under Review (SPUR) report on a biweekly basis. This report is now being sent electronically as well as a hard copy. This report is composed of the UES log sheet indicating the proposals sent out, the names of the evaluators to whom the proposals were sent, the dates the proposals were mailed, the tickle date, any necessary comments, and the date the reviews were received. This allows the Program Managers to have a current listing of all proposal activity.

B. Contractor/Program Reviews

1. The first program review was joint and entitled Molecular Dynamics (MD) and High Energy Density Matter (HEDM). It was held 17-22 May 1998 at the Hyatt Regency in Monterey, CA. Of the 143 attendees, 58 were speakers. These two meetings were held consecutively to stimulate interactions between program participants, and to expose AFOSR investigators to the wide range of topics being addressed in Air Force programs. Recent advances and accomplishments of the program were outlined at these

meetings. UES acquired the meeting site and made all arrangements for the meeting including meals and audio visual equipment. UES also provided on-site support and one advisor for the MD portion of the meeting.

Dr. Michael Berman, Program Manager

2. The second program review was a joint AFOSR/ONR/NSF **Tribology** review encompassing a wide range of topics: lubricants, wear resistant coatings, synthesis, characterization, modeling, simulations, metals, ceramics, polymers, etc. It was a broadbrush approach to the area and represented most of the tribology funded in the USA. This joint meeting brought together in one place all PI's funded in tribology to allow for crossfertilization to take place. It also allowed the program managers to look at the programs as a whole, assess impacts, and possible new directions needed. It was deemed invaluable to the program managers as a source of what research the community is performing. This joint meeting provided participants insight into what the other participants are contributing and how and provided the opportunity for new collaborations between attendees. It was held 22-25 June 1998 at the Lowes Annapolis Hotel in Annapolis, MD. Of the 61 attendees, 49 were speakers.

Major Hugh De Long, Program Manager

3. The third program review was **MURI and Durable Coatings.** It was held 11-22 January 1999 at Hawk's Cay Resort and Marina in Duck Key, Florida. There were 78 in attendance of which 59 were speakers. UES provided travel and per diem for 6 reviewers. UES also provided on-site support, made all arrangements for the meeting including meals and audio visual equipment.

Major Hugh De Long, Program Manager

C. Workshops

- 1. The first workshop was a **Night Ops Working Group** workshop. It was held at Charleston AFB, SC on 28-29 May 1998. UES provided 9 advisors for the subject workshop and made arrangements for coffee breaks.
- Dr. Genevieve Haddad, Program Manager
- 2. The second workshop was entitled **Polymer Composites**, and was held at the Anaheim Hilton & Towers in Anaheim, CA on 5 June 1998. UES made arrangements for the meeting location, audio visual and coffee breaks. *Dr. Charles Lee, Program Manager*.
- 3. The third workshop was entitled **POSS Polymers** and was held at Sommerfield Suites, El Segundo, CA on 16 February 1999. Approximately 8-12 were in attendance. UES made arrangements for the meeting location, audio visual and beverages. *Dr. Mike Berman, Program Manager*

D. Panel Meeting

The **Phase I STTR** panel meeting was held 18-19 February 1999 at Holiday Inn I 675 in Fairborn, OH. The purpose of this workshop was to hold a Phase I progress review to facilitate selection of Phase I efforts for submitting Phase II proposals for Phase II competition. Adhesives, flexible electronics and photonics were reviewed. There were ten presenters. UES made arrangements for the meeting room, audio visual equipment and coffee breaks.

Dr. Charles Lee, Program Manager

E. Advisors

In addition to advisors provided for Program Reviews, Workshops and Panel Meetings, UES provided travel, per diem and in many cases, honorarium for the following advisors:

Peter Stang and Frank Bates, Nanostructures, University of Southern California, Berkeley, CA, 9-10 March 1998.

Pat Hagans, Corrosion Symposium, Electrochemical Society Meeting, San Diego, CA, 3-8 May 1998.

Eileen Kowler and David Kieras, Advisors on Human Performance, George Mason University, Fairfax, VA, 26 May 1998.

Joan Fuller, European Research Conference on Molten Salts, Porquerolles, FR, 27 Jun – 3 Jul 1998.

Torbjorn Akerstedt, **AFOSR PRET Meeting**, Brigham & Women's Hospital, Boston, MA, 17 Jul 1998.

Ray Taylor, Workshop on Advanced Metal Finishing Techniques for Aerospace Applications, Keystone Resort, Keystone, CO, 23-28 Aug 1998.

Stephen Davis, Workshop on Chemical Laser, Albuquerque, NM, 16-18 Sep 1998.

Willard Larkin, Technical Advisor to AFOSR, Arlington, VA, 1 Oct – 31 Dec 1998.

Roger Brooks and Richard Goris, AFOSR MURI Workshop in Infrared Biosensors, University of Texas, Austin, TX, 2-3 February 1999.

SUMMARY

UES is pleased to continue to perform the specific tasks assigned to them in accordance with provisions of the contract. Participants will continue to be Dr. Thomas Eggemeier as Program Manager, Judith M. Flory, Program Administrative Manager, Donna Tinley, Assistant Program Administrator and Ann Corbitt as Program Assistant. UES personnel appreciate the opportunity to be of service to AFOSR in this interesting and worthwhile program.

LIST OF APPENDICES

Breakdown of Research Proposals by Program Manager

Program for Molecular Dynamics Contractor's Meeting, Naval Postgraduate School and Hyatt Regency Monterey, Monterey, CA, 17-20 May 1998

Program for High Energy Density Matter Contractor's Meeting, Naval Postgraduate School and Hyatt Regency Monterey, Monterey, CA, 20-22 May 1998

Program for Night Operations Working Group Site Visit, 437th Airlift Wing, Charleston AFB, SC, 27-29 May 1998

Program for AFOSR/ONR/NSF Tribology Program Review, Lowes Annapolis Hotel, Annapolis, MD, 22-25 June 1998

Programs for MURI and Durable Coatings Program Reviews, Hawk's Cay Resort and Marina, Duck Key, Florida, 11-21 January 1999

Program for STTR Program Review, Holiday Inn Conference Center I-675, Fairborn, OH, 18-19 February 1999

BREAKDOWN OF RESEARCH PROPOSALS BY PROGRAM MANAGER

PROGRAM MANAGER	NO. OF PROPOSALS
Berman	17
De Long	6
Kozumbo	5
Larkin	1
Lee	19
Roach	8
Tangney	10

1998 Molecular Dynamics Contractor's Meeting Naval Postgraduate School and Hyatt Regency Monterey Monterey, CA 17-20 May 1998

Sunday, 17 May 1998

5:00 - 7:00 PM	Registration
7:00 - 7:15 PM	Introductory Remarks Dr. Michael Berman, AFOSR
7:15 - 7:45 PM	Ion Processes in the Upper Atmospheric and Space Environments Dr. Rainer A. Dressler, AFRL, Hanscom AFB
7:45 - 8:15 PM	Potential Energy Surfaces and Their Dynamic Implications Dr. Keiji Morokuma, Emory University
8:15 - 8:45 PM	Reactive Scattering of Atomic Oxygen on Hydrocarbon Surfaces Dr. Timothy K. Minton, Montana State University
8:45 - 9:00 PM	Numerical Spectral Pattern Recognition Dr. Matthew P. Jacobson, Massachusetts Institute of Technology
Monday, 18 May 1998	
Monday, 18 May 1998 8:45 - 9:15 AM	Program Overview and Update Dr. Michael Berman, AFOSR
•	·
8:45 - 9:15 AM	Dr. Michael Berman, AFOSR Reactivity of Air Plasma Ions with Hydrocarbon Fuel Components
8:45 - 9:15 AM 9:15 - 9:45 AM	Dr. Michael Berman, AFOSR Reactivity of Air Plasma Ions with Hydrocarbon Fuel Components Dr. Robert A. Morris, AFRL, Hanscom AFB State-Resolved Ion Reactions and Ultrafast Photoelectron Spectroscopy

Monday, 18 May 1998 (Cont'd)

11:15 - 11:45 AM	Dynamics of Hypervelocity Collisions at the Gas/Surface Interface Dr. Dennis C. Jacobs, University of Notre Dame		
11:45 AM - 12:15 PM	Cluster Ion Beam Deposition for Study of Solid-Solid Interactions Dr. Scott L. Anderson, University of Utah		
12:15 - 2:00 PM	Lunch		
2:00 - 2:30 PM	Molecular Beam Studies of Reactions between Stratospheric Gases and Supercooled Sulfuric Acid Dr. Gilbert M. Nathanson, University of Wisconsin		
2:30 - 3:00 PM	H ₂ O Adsorption and Desorption Kinetics on α-Al ₂ O ₃ (0001) Dr. Steven M. George, University of Colorado		
3:00 - 3:30 PM	First Principles Studies of Metal and Metal Oxide Surfaces Dr. Emily A. Carter, University of California		
3:30 - 4:00 PM	Efficient Optimization of the Geometries of Large Molecules in Internal Coordinates Dr. Peter Pulay, University of Arkansas		
	Dr. 1 eter 1 utdy, Oniversity of Arkansas		
7:30 PM	Poster Session		
7:30 PM Tuesday, 19 May 1998			
Tuesday, 19 May 1998	Poster Session Rotational and Vibrational Nonequilibrium Effects in Infrared Atmospheric Backgrounds		
Tuesday, 19 May 1998 8:45 - 9:15 AM	Poster Session Rotational and Vibrational Nonequilibrium Effects in Infrared Atmospheric Backgrounds Dr. Steven J. Lipson, AFRL, Hanscom AFB Gateway Mediated Intersystem Crossing in Acetylene		
Tuesday, 19 May 1998 8:45 - 9:15 AM 9:15 - 9:45 AM	Rotational and Vibrational Nonequilibrium Effects in Infrared Atmospheric Backgrounds Dr. Steven J. Lipson, AFRL, Hanscom AFB Gateway Mediated Intersystem Crossing in Acetylene Dr. Robert W. Field, Massachusetts Institute of Technology Direct IR Laser Absorption Studies of Radical Kinetics and State-To-State Reactive Scattering Dynamics		

Tuesday, 19 May 1998 (Cont'd)

11:15 - 11:45 AM	Intramolecular Energy Transfer and Bond-Selected Photodissociation Dynamics Dr. F. Fleming Crim, University of Wisconsin - Madison
11:45 AM - 12:15 PM	New and Improved Propellants and Propulsion Techniques for Rockets and Satellites Dr. Patrick G. Carrick, AFRL, Edwards AFB
12:15 - 2:00 PM	Lunch
2:00 - 2:30 PM	Cavity Ringdown Laser Absorption Spectroscopy Dr. Richard J. Saykally, University of California, Berkeley
2:30 - 3:00 PM	Vibronic Coherences and The Dissection of Elementary Steps in Chemical Dynamics in Condensed Media Dr. V. Ara Apkarian, University of California, Irvine
3:00 - 3:30 PM	Interfacing Electronic Structure Theory with Dynamics Dr. Mark S. Gordon, Iowa State University
3:30 - 4:00 PM	The Generation, Conformations and Energetics of Exotic Species in The Gas Phase: Oligomers of Synthetic Polymers and Transition Metal Benzene Clusters Dr. Michael T. Bowers, University of California at Santa Barbara
7:30 - 8:00 PM	I(² P _{1/2})+O ₂ : Studies of Low Temperature Electronic Energy Transfer and Nuclear Spin State Changing Collisions Dr. Michael C. Heaven, Emory University
8:00 - 8:30 PM	Interactions of HCl(v=2) with MgO(100) Drs. Curt Wittig and Hanna Reisler, University of Southern California
8:30 - 9:00 PM	Surface Scattering of Highly Vibrationally Excited Molecules Dr. Alec Wodtke, University of California at Santa Barbara
Wednesday, 20 May 1998	
8:30 - 9:00 AM	Optical Excitation, Ionization and Reactive Dynamics of Molecular Clusters Dr. Albert W. Castleman, Jr., The Pennsylvania State University

Wednesday, 20 May 1998 (Cont'd)

9:00 - 9:30 AM	Spectroscopy and Dynamics in Novel Metal-Containing Clusters Dr. Michael A. Duncan, University of Georgia
9:30 - 10:00 AM	Linear Scaling Density Functional Methods with Periodic Boundary Conditions Dr. Gustavo E. Scuseria, Rice University
10:00 - 10:30 AM	Break
10:30 - 11:00 AM	Collective Electronic Excitations in Nonlinear Spectroscopy of Conjugated and Aggregated Molecules Dr. Shaul Mukamel, University of Rochester
11:00 - 11:30 AM	Two-Color Laser Desorption-Ionization Time-of-Flight Mass Analysis of Aerosols Drs. Roger E. Miller and Tomas Baer, University of North Carolina
11:30 AM - 12:00 PM	Vibrational Dynamics in Supercritical Fluids Dr. Michael D. Fayer, Stanford University
12:00 - 12:30 PM	Ultrafast Vibrational Dynamics in Condensed Phases Dr. Dana D. Dlott, University of Illinois at Urbana Champaign
1:00 PM	BBQ at Hyatt Regency Monterey

1998 High Energy Density Matter Contractor's Meeting Naval Postgraduate School and Hyatt Regency Monterey Monterey, CA 20-22 May 1998

Wednesday, 20 May 1998

1:00 PM

BBQ at Hyatt Regency Monterey

7:00 PM

Poster Session

Thursday, 21 May 1998	
7:45 - 8:45 AM	Registration
8:45 - 9:15 AM	Introductory Remarks: Dr. Michael Berman, AFOSR
9:15 - 9:45 AM	Air Force Research Lab Perspective on Advanced Propulsion Dr. Stephen L. Rodgers, AFRL, Edwards AFB
9:45 - 10:15 AM	Solid Parahydrogen Dr. Mario E. Fajardo, AFRL, Edwards AFB
10:15 - 10:45 AM	Break
10:45 - 11:15 AM	Insights into the Stability and Synthesis of High Energy Density Matter through Largescale Computer Simulation Dr. Gregory A. Voth, University of Utah
11:15 - 11:45 AM	Stability and Mobility of O Atoms and Ozone in an Oxygen Matrix Dr. Richard A. Copeland, SRI Internatinal
11:45 AM- 12:15 PM	Three-Phase Modeling of Frozen-Ozone Combustion Dr. Martin S. Miller, Army Research Laboratory
12:15 - 2:00 PM	Lunch
2:00 - 2:30 PM	Spectroscopic Characterization of Non-bonding Interactions of the Aluminum Atom

Dr. Paul J. Dagdigian, Johns Hopkins University

Thursday, 21 May 1998 (Cont'd)

2:30 - 3:00 PM	Probing Barriers to the Aggregation of Light Metal Atoms Using Helium Cluster Isolation Spectroscopy Dr. Giacinto Scoles, Princeton University
3:00 - 3:30 PM	Theoretical Investigations of HEDM Dr. Jeffrey A. Sheehy, AFRL, Edwards AFB
3:30 - 4:00 PM	Break
4:00 - 4:30 PM	Spectral Theory of Adiabatic Electronic Schrödinger Eigenstates: Theory and Implementation for Atomic Aggregates Dr. Peter W. Langhoff, AFRL, Edwards AFB
4:30 - 5:00 PM	Quantitative Analysis of the Condensation of B_JC_{nJ} Clusters (n = 2-12, J = 0, 1, 2) in Solid Argon Dr. C. William Larson, AFRL, Edwards AFB
5:00 - 5:30 PM	Advanced Cryogenic Solid Hybrid Rocket Engine Developments for HEDM and Non-HEDM Demonstrations - A 1998 Status Report Dr. Eric E. Rice, Orbital Technologies Corporation
Friday, 22 May 1998	
8:45 - 9:15 AM	Does the O ₄ Molecule Exist? Dr. Rodney J. Bartlett, University of Florida
8:45 - 9:15 AM	Dr. Rodney J. Bartlett, University of Florida Extra-High Energy Oxidizers and Fuels
8:45 - 9:15 AM 9:15 - 9:45 AM	Dr. Rodney J. Bartlett, University of Florida Extra-High Energy Oxidizers and Fuels Dr. Robert J. Schmitt, SRI International An Overview of the FOA Energetic Materials
8:45 - 9:15 AM 9:15 - 9:45 AM 9:45 - 10:15 AM	Dr. Rodney J. Bartlett, University of Florida Extra-High Energy Oxidizers and Fuels Dr. Robert J. Schmitt, SRI International An Overview of the FOA Energetic Materials Dr. Henric Östmark, FOA
8:45 - 9:15 AM 9:15 - 9:45 AM 9:45 - 10:15 AM 10:15 - 10:45 AM	Dr. Rodney J. Bartlett, University of Florida Extra-High Energy Oxidizers and Fuels Dr. Robert J. Schmitt, SRI International An Overview of the FOA Energetic Materials Dr. Henric Östmark, FOA Break Reaction Field Cavity Optimization

Friday, 22 May 1998 (Cont'd)

12:15 - 2:00 PM	Lunch
2:00 - 2:30 PM	Development of New Energetic Materials for Advanced Solid Rocket Propellants Dr. Lou Cannizzo, Thiokol Corporation
2:30 - 3:00 PM	Synthesis of High-Energy Density Materials Based on Strained-Ring Compounds Dr. William P. Dailey, University of Pennsylvania
3:00 - 3:30 PM	Theory and Synthesis of New High Energy Density Materials Dr. Karl O. Christe, Raytheon STX
3:30 - 4:00 PM	Pseudochalcogenide Nitrite and Nitrate Analogues Dr. D. Scott Bohle, University of Wyoming
4:00 PM	Closing Remarks, adjourn Dr. Michael Berman, AFOSR

179NERARY

Night Operations Working Group Site Visit 437TH AIRLIFT WING CHARLESTON AFB SC

27-29 MAY 1998

Current as of 6 May 1998

Charleston AFB POC:

Lt. Col. Byron Hepburn

Office: 803-963-5829 Home: 803-884-6257

Billeting:

Charleston AFB Protocol

Comm: (803) 963-3879 DSN: 673-3879 (Direct Line)

Wednesday, 27 May 1998

PM Arrival at Leisure/Check in at Charleston House Billeting, Bldg 322

Thursday, 28 May 1998		
0715	Meet in Charleston House (Billeting) Lobby, Bldg # 322 (Lt Col Hepburn and SSgt Pace to greet and pickup visitors)	
0730	Continental Breakfast in Support Group Conference Room at Headquarters Bldg	
0800-0830	Welcome from Lt Col Hepburn and 437 $^{\text{th}}$ Airlift Wing Vice Commander Colonel Norris Briefings; Team Charleston, C-17, and SOLL Π	
0830-0900	Circadian and Metabolic Modulation of Human Vision Robert Barlow, Jr., State University of New York	
0900-0930	Initiatives from Chronobiology and Circadian Medicine to Maximize Military Readiness Charles A. Czeisler, Brigham and Women's Hospital	
0930-1000	New Developments in Identifying the Cumulative Effects of Sleep Restriction David F. Dinges, University of Pennsylvania, School of Medicine	
1000-1030	Break	

1030-1100	Pharmacological Countermeasures for Physiological Sleepiness: Insights from Pre-Clinic Studies Dale M. Edgar, Stanford University, School of Medicine
1100-1130	Fatigue and Night Operations Jonathan French, AL/CFTO, Brooks Air Force Base
1130-1200	Collision Avoidance and Target Engagement David M. Regan, York University
1200-1300	Lunch at Charleston Club (Buffet)
1315-1415	Tour C-17 Simulator
1430-1515	C-141 SOFI Aircraft Tour (Col Dale Kissinger)
1530-1600	Life Support Visit (Night Vision Goggle Demo)
1615-1715	Free Time
1730	Pickup at Charleston House for dinner with Brig Gen Steve Roser and Mrs. Linda Roser. Dress: Jacket and Tie for gentlemen, Summer Dress for ladies.
1800	Cocktails at Charleston Place, Downtown in Hospitality Suite 2L
1900-2100	Dinner

Friday,	29	May	1998
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0700-0715	Pickup at Charleston House by Lt Col Hepburn and SSgt Pace (Please checkout prior to departure) Dress: Flight suits for active duty, Casual wear for civilians
0730-0800	Continental Breakfast in DV lounge at the Passenger Terminal
0800	Depart for aircraft
0900-1400	Orientation flight (Box Lunches)
1400-1430	Meeting Wrap Up, DV lounge Passenger Terminal

POCs: Lt Col Byron Hepburn, home (803) 884-6257 and SSgt Sharon Pace, office (803) 963-5829

AFOSR/ONR/NSF Tribology Program Review Lowes Annapolis Hotel Annapolis, MD 22-25 June 1998

Monday, 22 June 1998

0730	Registration/Continental Breakfast
0820	Introduction Dr. Hugh De Long, AFOSR, Dr. Peter Schmidt, ONR, and Dr. Jorn Larsen-Basse
0830	Nanotribology, Nanomechanics and New Molecular Probes Charles M. Lieber, Harvard University
0900	Solid Lubricant Replenishment Systems Thierry A. Blanchet, Rensselaer Polytechnic Institute
0930	Design of Tribological Properties via Self-Assembling Nanocomposite Molecular Films Vladimir V. Tsukruk, Western Michigan University
1000	Break
1015	Nanotribological Studies of Bulk Ceramic Materials. Multilayered Thin Films, and Liquid Lubricant Films Bharat Bhushan, The Ohio State University
1045	Surface Treatments for Probing of Tribological State Variables, Ursula Gibson, Dartmouth College
1115	Theoretical Simulations of Low-Dimensional Materials J. W. Mintmire, C. T. White, Naval Research Laboratory
1145	Friction Control in Thin Film Lubrication Jianping Gao, W. D. Luedtke, <u>Uzi Landman</u> , Georgia Institute of Technology
1215	Lunch

Monday, 22 June 1998 (Cont'd)

1400	Magnetron Sputtered Quasicrystalline Coatings - A Breakthrough for Thin Film Applications Larry L. Fehrenbacher, Technology Assessment & Transfer, Inc.
1425	Tribological Behavior of Sputtered Quasicrystalline Alloys in Extreme Environments A Preliminary Study Michael N. Gardos, Raytheon Systems Company
1450	Frictional Properties of Quasicrystalline Surface Andrew J. Gellman, Carnegie Mellon University
1515	Investigation of Quasicrystal Coatings for Friction and Wear Control in Extreme Environments J. S. Zabinski, N. A. Pierce, S. V. Prasad, AFRL/MLBT
1540	Break
1555	The Surface Chemistry and Tribology of Metal Carbides and Nitrides Scott S. Perry, University of Houston, Steve Didziulis, The Aerospace Corporation
1625	Preparation of Carbon Films on SiC by High Temperature Chlorination M. McNallan, D. Ersoy, Y. Gogotsi, University of Illinois at Chicago

Tuesday, 23 June 1998

0730	Continental Breakfast
0830	Kelvin Probe Measurements Applied to Bearing Diagnostics <u>Steven Danyluk</u> , YeYuan Yang, Georgia Institute of Technology
0900	Sliding Friction and Wear of Selected Aluminum-Based Bearing Alloys and Preliminary Results Using an <i>In Situ</i> Kelvin Probe to Monitor Changes in Surface Condition K. Lepper, J. Chashechkina, T. Kasai, A. Zharin, and D. A. Rigney, The Ohio State University
0930	Mixing of Materials During Sliding with and Without Lubrication <u>John L. Young, Jr.</u> , D. Kuhlmann-Wilsdorf, and Robert Hull, University of Virginia

Tuesday, 23 June 1998 (Cont'd)

1000	Break
1015	Debris Denting, Spall Initiation and Propagation in Lubricated Contacts Farshid Sadeghi, Purdue University
1045	Deformation Behavior of Thin Liquid Films at Elevated Pressure Scott Bair, Georgia Institute of Technology
1115	Transient Behavior of Rotary Lip Seals Richard F. Salant, Georgia Institute of Technology
1145	Recent Advances in Experimental Techniques for Investigating High Speed Friction Vikas Prakash, Case Western Reserve University
1215	Lunch
1400	Spectroscopic Probes of Boundary Lubricants and Perfluoropolyethers Steve Granick, University of Illinois
1430	In Situ Laser Spectroscopic Studies of Boundary Lubricant Films Gerold A. Willing, Sangkwon Park, Ronald D. Neuman, Auburn University
1500	Characterization of Surface Reactions on Iron in the Presence of Perfluoropolyalkylether Lubricants at Elevated Temperatures Jeffrey H. Sanders, AFRL MLBT
1530	Break
1545	Tribological Surface Chemistry Andrew J. Gellman, Carnegie Mellon University
1615	Free Vibration Analysis of PZT Glide Heads during Disk/Head Interfacial Contacts Alex Y. Tsay, I. Y. (Steve) Shen, University of Washington, CP. Roger Ku, IBM, Bruno Marchon, Seagate Technology
1645	Structural Analysis of MEMS Pressure Sensors for Disk/Head Interfacial Contact Application <u>Liwei Lin</u> , Yen-Wen Lu, The University of Michigan

Wednesday, 24 June 1998

0730	Continental Breakfast
0830	Lubricative Gas-Phase Reactions of Silicon and Polycrystalline Diamond with Dry/Wet Hydrogen and Dry Oxygen for MEMS Applications Michael N. Gardos, Raytheon Systems Company
0900	Development of a New, Reactive Potential Energy Function to Study the Tribology of Hydrocarbon Systems Judith A. Harrison, United States Naval Academy
0930	Nano-Composite Coatings Consisting of Carbides, Diamond-Like Carbon, and Dichalcogenates for Aerospace Tribology A. A. Voevodin, J. P. O'Neill, J. S. Zabinski, AFRL MLBT
1000	Break
1015	Nanotribology of Vapor-Phase Lubricants Jacqueline Krim, North Carolina State University
1045	Vapor Lubrication Mechanisms: Heat Generation in High Speed Rolling Element Bearings Nelson H. Forster, Lewis Rosado, Garry D. Givan, AFRL PRSL
1115	Studies of the Effect of PVD TiN Coatings on the Rolling Contact Fatigue Life L. M. Keer and YW. Chung, Northwestern University
1145	Thermal-Tribological Designs of Mechanical Elements <u>Oian (Jane) Wang</u> and Y. Cao, Florida International University
1215	Lunch
1400	In Vivo Raman Tribometry: Real-time Analysis of Friction, Wear and Third Body Processes I. L. Singer, K. J. Wahl, Naval Research Laboratory
1430	Sol-Gel Derived, Nanostructure Dioxide Lubricant Coatings Douglas J. Taylor, <u>Stuart T. Schwab</u> , Patrick F. Fleig, TPL, Incorporated, Richard A. Page, Southwest Research Institute

Wednesday, 24 June 1998 (Cont'd)

1500	In Situ Studies of the Nucleation and Growth of Cubic Boron Nitride L. D. Marks, E. Bengu, C. Collazo-Davila, Northwestern University
1530	Break
1545	Atomistic Simulations of Adhesive Interactions with α -Alumina and Hydroxylated α -Alumina Surfaces William L. Hase, Wayne State University
1615	Friction and Adhesion Studies Using the Surface Forces Apparatus Jacob Israelachvili, Cyrus Safinya, Yuval Golan, University of California at Santa Barbara
1645	Adhesion studies: Liquid Capillarity and Micro-scale Impact Dr. Jeffrey L. Streator, Georgia Institute of Technology

Thursday, 25 June 1998

0730	Continental Breakfast
0830	Predicting Fracture Behavior of Polycrystalline Covalent Ceramics Using a Hybrid of Computational Methods <u>Donald W. Brenner</u> , Olga A. Shenderova, North Carolina State University
0900	Adaptive Wide Temperature Solid Lubricant Films by Magnetron Sputtering and Ion Beam Assisted Deposition Larry L. Fehrenbacher, Technology Assessment Transfer, Inc.
0930	Lubrication Mechanisms in Zinc Oxide Coatings <u>J. S. Zabinski</u> , N. Pierce, J. Nainaparampil, S. V. Prasad, AFRL MLBT
1000	Break
1015	Modeling the Interactions Between Compressed Polymer Surfaces Anna (*. Balazs, University of Pittsburgh
1045	In Situ Investigation of the Influence of a Mechanical Load on the Orientation of Organic Monolayers with Second Harmonic Generation F. Eisert, M. Gurka, M. Buck, and M. Grunze, Institut für Angewandte Physikalische ('hemie

Thursday, 25 June 1998 (Cont'd)

1115	A Robust, Deterministic Model for Thermal Mixed-Film Lubrication Liming Chang, Penn State University
1145	The Nature of Tribochemistry & It's Effect on Lubrication Stephen Hsu, University of Maryland/(NIST)
1215	Lunch
1400	An Investigation of Certain Dynamic Instabilities in Dry Sliding George G. Adams, Northeastern University
1430	Density-Functional Chemical Dynamics with Fractional Occupation Numbers, Brett I. Dunlap, Naval Research Laboratory
1500	An Integrated Study on Conformal Contacts Qian (Jane) Wang, Florida International University
1530	Break
1545	Integrated Diagnostics Richard S. Cowan, Georgia Institute of Technology
1615	Chemical Imaging and Molecular Diagnostics Using Optical Spectroscopy Dor Ben-Amotz, Purdue University
1645	Modeling of Lubrication Breakdown of Sliding Contacts Dr. Si. C. Lee, The Ohio State University

Agenda

Mechanism of Al Alloy Corrosion and the Role of Chromate Inhibitors MURI Program Review

January 11-12,1999

Monday, January 11, 1999		
9:00 - 9:30	Overview (Frankel)	
9:30 - 10:30	Surface Science Aspects of Chromate Inhibition (Clayton/Halada)	
10:30 - 10:45	break	
10:45 - 11:45	XANES and Electrochemical Studies of Chromate Conversion Coatings and Pure Aluminum, (Isaacs)	
11:45 - 1:00	lunch	
1:00 - 2:00	Chromate Inhibitors in Paint Systems (Granata)	
2:00 - 3:00	Filiform Corrosion of Al Alloys (Stratmann)	
Tuesday, January 12, 1999		
9:00 - 10:00	Structure and Dynamics of Chromate Films on AA2024-T3 (McCreery)	
10:00 - 10:30	break	
10:30 - 11:30	The Effect of Chromate on Localized Dissolution of Alloys (Frankel)	
11:30 - 1:00	lunch	
1:00 - 2:00	Mechanism of Al Alloy Corrosion and the Role of Chromate Inhibitors – Ionic and Intermetalic Aspects (Kendig)	
2:00 - 3:00	Summary (Frankel)	

Agenda

MURI: Prevention of Corrosion in Structural Aluminum Alloys

Wednesday, January 13, 1999

Morning session: 9:00am - 11:30 am

9:00 am

"Prevention of Corrosion in Structural Aluminum Alloys"

K. Sieradzki, Arizona State University

9:40 am

"Corrosion-Induced Nanostructure and Morphology of Aluminum Alloys"

R. Carpenter, Arizona State University

Break 10:20 am - 10:35 am

10:40 am

"Electrochemistry of Cu Redistribution During Corrosion of Aluminum Alloys" N. Dimitrov, *Arizona State University*

Lunch 11:30 am - 12:55 pm

Afternoon session 1:00 pm - 3:00 pm

1:00 pm

"Mechanisms of particle removal and copper redistribution on 2024 surfaces" A. Davenport, *Univ. of Manchester/Univ. of Birmingham*

1:40 pm

Computer Simulations of Aluminum Alloy Corrosion J. Erlebacher, *Harvard Univ*.

2:20 pm

Protecting Aluminum Alloys Against Copper: The Future

R. Newman, UMIST



AGENDA FOR JANUARY 14, 1999 URI REVIEW – North Dakota State University

TIME	TOPIC	SPEAKER
9:00	Introduction & Project Summary	Gordon Bierwagen
9:20	Improved EIS Instrumentation Design	David Farden
10:30	BREAK	
10:50	Sample Handling & Electrochemical Data	Gordon Bierwagen
11:30	AFM Results & Implications	Dennis Tallman
12:00	LUNCH	
12:45 PM	SVET & Conductive Polymer Results and Interpretation	Dennis Tallman
1:15	Spectroscopic Results & Interpretation	Marek Urban
2:30	Conclusions and Future Work	Gordon Bierwagen

1999 Durable Coatings Program Review Hawk's Cay Resort and Marina Osprey Room Duck Key, Florida 15 January 1999

Friday, 15 January 1999

riday, 15 gandary 1999	
7:25 - 8:25 AM	Registration/Continental Breakfast
8:25 - 8:30 AM	Introductory Remarks Dr. Charles Lee, AFOSR
8:30 - 9:15 AM	UniCoat Airplane Coatings System: Corrosion Resistant Ceramer Coatings Dr. Mark D. Soucek, North Dakota State University
9:15 - 10:00 AM	Durable Multilayer Coatings Dr. Thomas Seery and Dr. Jeff Koberstein, University of Connecticut
10:00 - 10:15 AM	Break
10:15 - 1100 AM	Characterization of Heterogeneous Regions in Polymer Coatings Dr. Dharmaraj Raghavan, Howard University
11:00 AM - 12:00 PM	Characterization of Aging-Induced Physical and Chemical Defects in Aircraft Long-Life Coating Systems Dr. Y. C. Jerry Jean and Dr. Thomas C. Sandreczki, University of Missouri-Kansas City
12:00 - 1:30 PM	Lunch
1:30 - 2:15 PM	Optical Imaging for Nondestructive Evaluation of Microstructure, Fracture, Delamation and Degradation in Multilayer Organic Coatings and Paints Dr. Paras N. Prasad, State University of New York at Buffalo
2:15 - 2:45 PM	Multi-Color Electrochromic Polyer Coatings Dr. John R. Reynolds, University of Florida
2:45 - 3:00 PM	Break

Friday, 15 January 1999 (Cont'd)

3:00 - 3:30 PM	Corrosion Protection of Aluminum and Aluminum Alloys Using Polyanilines Dr. Arthur J. Epstein, The Ohio State University
3:30 - 4:30 PM	Coating Technology for Long Term Air Force Goals Dr. Fred E. Arnold, AFRL MLBP, WPAFB
4:30 PM	Adjourn



NDE-MURI Review 1999

January 18 - 19, 1999 Location: Hawk's Cay Resort Duck Key, Florida

Monday, January 18, 1999

Overview

9:00 – 10:00 A.M. Overview of the NDE-MURI Program (Matikas)

Quantification of LCF/HCF Damage

10:00 – 10:15 A.M.	Characterization of Fatigue Damage Accumulation (Maurer)
10:15 - 10:30 A.M.	BREAK
10:30 - 11:00 A.M.	Real - Time Monitoring of Fatigue Damage through Nonlinear Acoustics (Sathish)
11:00 - 11:30 A.M.	LCF/HCF Interaction Using a 20 kHz HCF Cell (Matikas)
11:30 - 1:00 P.M.	LUNCH
1:00 - 1:15 A.M.	Temperature Monitoring of Fatigue Damage (Meyendorf)
1:15 - 2:00 P.M.	Early Detection of Fatigue Cracks - Eddy Current and Laser-Ultrasonic Techniques (Nagy)
2:00 - 2:30 P.M.	Fatigue Crack Detection via Holography and Interferometry of SAW (Blackshire)
2:30 - 2:50 P.M.	Image Processing for Phase-Stepped Interferometry and Resolution Enhancement (Hardie)
2:50 - 3:00 P.M.	Summary and Concluding Remarks
3:00 P.M.	Adjourn

Tuesday, January 19, 1999

Fretting Fatigue Damage Characterization

9:00 - 9:30 A.M.	Prediction of Fatigue Crack Instability through Surface Nondestructive Characterization (Matikas)
9:30 - 10:00 A.M.	Interface Contact Conditions in Fretting Fatigue - Fretting Maps and Temperature Rise (Nicolaou)
10:00 - 10:30 A.M.	BREAK
10:30 - 10:45 A.M.	Nano-scale NDE for Elastic Property Imaging (Sathish)
10:45 - 11:15 A.M.	Characterization of Fretting Fatigue Damage on Ti-6Al-4V Alloys (Nicolaou)
11:15 - 1:00 P.M.	LUNCH

Corrosion Characterization

1:00 -	1:45 P.M.	Pitting Initiation and Coating Degradation – Developing Corrosion and NDE Metrics (Khobaib)
1:45 -	2:30 P.M.	Microradiographic Detection of Corrosion (Rokhlin)
2:30 -	2:45 A.M	NDE of Protective Coatings (Mevendorf)
2:45 -	3:00 P.M.	Summary and Concluding Remarks
	3:00 P.M.	Adjourn

Agenda

3rd Annual Review of AFOSR MURI "Nanoscale Devices and Novel Engineered Materials" University of Florida

Monitor: Maj. H.C. DeLong, Ph.D.

W	ed	nes	day	
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January 20, 1999

Location: Hawk's Cay Resort, Marathon, FL

9:00-9:20 am

Welcome and Overview; Program Goals and Achievements

S.J. Pearton (MSE/UF)

Novel Engineered Materials and Properties

9:20-10:00 am	Mechanical Properties of Nanostructured Materials S.A. Syed Asif (NRL)
10:00-10:30 am 10:30-11:00 am	Nanostructured Display Materials, P.H. Holloway (MSE/UF) Coffee Break
New Directions	Magnetotransport - charge, frequency and noise properties

TEW Directions	
11:00-11:15 am	Magnetotransport - charge, frequency and noise properties
	A.F. Hebard (Physics/UF)
11:15-11:30 am	Integration of Magnetic Materials and Semiconductors
	F. Ren (Chem. Eng./UF)
11:30-12:00 am	Deposition and Etching of Ferromagnetic Particles in a Non Magnetic
	Matrix, A.C. Kummel (Chem/UCSD)
12:00-1:30pm	Lunch
1:30-2:00 pm	Pulsed Laser Deposition of CMR Oxides, R.K. Singh (MSE/UF)
2:00-3:00 pm	Discussion (all)

Thursday

January 21, 1999

Submicron Magnetic Structures: Deposition, Processing and Theory

9:00-9:15 am	Overview and Accomplishments, S.J. Pearton (MSE/UF)
9:15-10:00 am	Physics of Length Scales in Magnetic and Superconducting
	Microstructures, I.K. Schuller (Physics/UCSD)
10:00-10:30 am	Integration of Magnetic Nanoparticles with 2-D Electron Systems
	S. von Molnar (Physics/FSU)
10:30-11:00 am	Coffee Break
11:00-11:30 am	Nanostructure Patterning and Transport Physics
	F. Sharifi (Physics/UF)
11:30-12:00 am	Ion Beam Deposited GMR Materials
	D. Temple and G.E. McGuire (MCNC)
12:00-1:30 pm	Lunch
1:30-2:00 am	Dry Etching of Magnetic Multilayers, S.J. Pearton (MSE/UF)
2:00-2:30 pm	Theory and Modelling of GMR, S. Hershfield (Physics/UF)
2:30-2:45 pm	Summary/Accomplishments, S.J. Pearton
2:45-3:30 pm	Discussion (all)

AFOSR STTR PROGRAM REVIEW 18-19 February 1999

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Holiday Inn Conference Center I-675 Patterson Room Fairborn, Ohio

Thurse	lay, 18 February (Adhesives)
0800	AdTech - Dielectric Relaxation Spectroscopy of Adhesively Bonded Joints
0840	Aspen Systems - Liquid Crystalline Adhesive with Zero Shrinkage
0920	Cornerstone - High-Performance Liquid Crystal Adhesives
1000	Break
1015	DACCO - Electrochemical Sensors for Nondestructive Evaluation of Adhesive Bonds
1055	PolyComp - Development of High Temperature Low Cure Shrinkage Adhesives
1135	Triton - High Temperature Low Viscosity Polyimide Adhesive
1215	End
<u>Friday</u>	19 February 1999 (Flexible Electronics and Photonics)
0830	AdTech - Flexible Electronics and Photonics
910	Materials Research Institute - Inkjet Printing of Flexible Circuits on Polymer Substrate
0950	Break
1010	Pacific Wave Inc Flexible Polymer Modulators for Large Conformal Antenna Arrays
1050	UNIAX - Polymer LEDs made from Monochromatic Red-Emitting Polymer/Rare Earth Blends
1130	End